

SEARCH REF.

Requester's Full Name: Cecilia J. ...

Art Unit: 16 24

2014-10-20 10:10:10

Serial Number: 7432 Date: 11/11/2010

Location (Bldg-Room): 84525 (Bldg-Rm) 29

Serial Number: 10395-74-3

Revised Patent Prepared (date): PAPER: D6

7. ANSWER TO QUESTION: If possible, please attach a copy of the cover sheet, chapter, and abstract or fill out the following:

Title of Invention: See Bib Data Sheet

Inventors (please provide full names):

Fastest Priority List

ještětá Yopliz:

It also provides a new framework for the analysis of the economic situation of the country, and a new basis for the development of the national economy. The new framework is based on the principle of the unity of the national economy, and the new basis is based on the principle of the unity of the national economy.

For Sequence Searching Only: Please include in parentheses the date of the last revision to the document.

See claims attached. Please do literature search and invent. name(s) react. Display results to show identification of source, and R¹, compound name & structure of identified compounds. Please do a CAS React search, specifying the starting materials and a product with the hydrozole substructure and a Lewis acid in the reaction. See previous search.

Please call just any agent.

STATE USE ONLY

Figure 1: Example of a \mathbb{Z}_2 -invariant

[Downloaded from ascelibrary.org by University of California, San Diego on 06/09/14](#)

SEARCHED _____

H.A. Fomberg et al. / *Journal of Macroeconomics* 25 (2003) 611–630

STJ 111

Средства на расходы: _____

4. $\frac{1}{2} \pi \leq \theta \leq \frac{3}{2} \pi$

— *Continued* —

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3. **ALPHACIN (C)**

Environ Monit Assess (2008) 142:111–124

Deleuze e Guattari definiscono l'Utopia come:

Fluency and

10.50 μm 297.00 cm^{-1} 610.00 cm^{-1}

File completed: _____

উপসংক্ষেপ:

[illegible]

Signature of Elected Board Member _____

Ref: 1

^a See footnote 1 for definition of variables.

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Opis:

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=> file registry
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FILE 'REGISTRY' ENTERED AT 10:17:11 ON 17 OCT 2008

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DICTIONARY FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5

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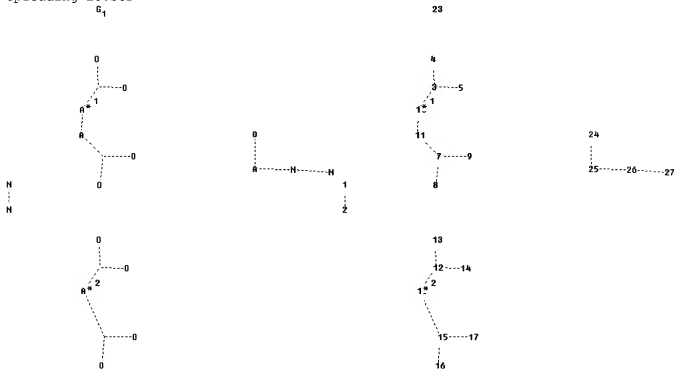
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Uploading L6.str



chain nodes :

3 4 5 7 8 9 12 13 14 15 16 17 23 24

ring/chain nodes :

1 2 10 11 18 25 26 27

chain bonds :

3-4 3-5 3-10 7-8 7-9 7-11 12-13 12-14 12-18 15-16 15-17 15-18 24-25

ring/chain bonds :

1-2 10-11 25-26 26-27

exact/norm bonds :

1-2 3-4 3-5 3-10 7-8 7-9 7-11 10-11 12-13 12-14 12-18 15-16 15-17 15-18

24-25

25-26 26-27

10/595943

G1:[*1],[*2]

Connectivity :

3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
7:3 E exact RC ring/chain 8:1 E exact RC ring/chain 9:1 E exact RC ring/chain
12:3 E exact RC ring/chain
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:3 E exact RC ring/chain
16:1

E exact RC ring/chain 17:1 E exact RC ring/chain 24:1 E exact RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS

fragments assigned product role:

containing 24

fragments assigned reactant/reagent role:

containing 1

containing 23

=> file caplus

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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17

FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

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<http://www.cas.org/legal/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L85

L73	643	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	LOPES C?/AU
L74	331	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	LOPES R?/AU
L75	368	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	CARDOSO J?/AU
L76	2399	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	SILVA J?/AU OR DA SILVA J?/AU
			OR DASILVA J?/AU			
L77	1104	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	FERREIRA L?/AU
L78	28	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L73 AND (L74 OR L75 OR L76 OR

```

L77)
L79      8 SEA FILE=CAPLUS ABB=ON  PLU=ON  L74 AND (L75 OR L76 OR L77)
L80      2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L75 AND (L76 OR L77)
L81     16 SEA FILE=CAPLUS ABB=ON  PLU=ON  L76 AND L77
L82      8 SEA FILE=CAPLUS ABB=ON  PLU=ON  L78 AND (L79 OR L80 OR L81)
L83      0 SEA FILE=CAPLUS ABB=ON  PLU=ON  L79 AND (L80 OR L81)
L84      0 SEA FILE=CAPLUS ABB=ON  PLU=ON  L80 AND L81
L85      8 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L82 OR L83 OR L84)

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=> d stat que L87
L6      STR

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L8      446 SEA FILE=CASREACT SSS FUL L6 ( 4732 REACTIONS)
L73     643 SEA FILE=CAPLUS ABB=ON  PLU=ON  LOPES C?/AU
L74     331 SEA FILE=CAPLUS ABB=ON  PLU=ON  LOPES R?/AU
L75     368 SEA FILE=CAPLUS ABB=ON  PLU=ON  CARDOSO J?/AU
L76     2399 SEA FILE=CAPLUS ABB=ON  PLU=ON  SILVA J?/AU OR DA SILVA J?/AU
        OR DASILVA J?/AU
L77     1104 SEA FILE=CAPLUS ABB=ON  PLU=ON  FERREIRA L?/AU
L86     446 SEA FILE=CAPLUS ABB=ON  PLU=ON  L8
L87      3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L86 AND (L73 OR L74 OR L75 OR
        L76 OR L77)

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=> file medline embase biosis wpix
FILE 'MEDLINE' ENTERED AT 10:17:32 ON 17 OCT 2008

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=> s L85
L88      4 L85

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=> file zcaplus
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FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17
FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> s L85 or L87

L89 10 L85 OR L87

=> dup rem L89 L88

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PROCESSING COMPLETED FOR L88
L90 11 DUP REM L89 L88 (3 DUPLICATES REMOVED)

ANSWERS '1-10' FROM FILE CAPLUS
ANSWER '11' FROM FILE MEDLINE

=> d ibib abs L90 1-10; d iall L90 11

L90 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2007:667806 CAPLUS Full-text
DOCUMENT NUMBER: 147:257498
TITLE: A new chemoselective synthesis of brombuterol
AUTHOR(S): Nery, Marcelo S.; Azevedo, Mariangela S.; Cardoso, Jari N.; Slana, Glaucia B. C.; Lopes, Rosângela S. C.; Lopes, Claudio C.
CORPORATE SOURCE: Departamento de Química Analítica, Instituto de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro, CEP 21949 900, Brazil
SOURCE: Synthesis (2007), (10), 1471-1474
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:257498
AB A practical method for the synthesis of brombuterol [1-(4-amino-3,5-dibromophenyl)-2-(tert-butylamino)ethanol] in high overall yield is described starting from 4'-aminoacetophenone using a new chemoselective route.
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:493567 CAPLUS Full-text
DOCUMENT NUMBER: 143:26622
TITLE: Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids
INVENTOR(S): Lopes, Claudio Cerqueira; Lopes, Rosângela Sabattini Capella; Cardoso, Jari Nobrega; Alves Da Silva, Jacqueline; Ferreira Gomes, Leticia
PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro-UFRJ, Brazil
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051870	A2	20050609	WO 2004-BR236	20041125
WO 2005051870	A3	20050707		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
BR 2003007864	A	20050705	BR 2003-7864	20031125
US 20070128680	A1	20070607	US 2006-595943	20060522

10/595943

PRIORITY APPLN. INFO.:

BR 2003-7864

A 20031125

WO 2004-BR236

W 20041125

OTHER SOURCE(S):

CASREACT 143:26622; MARPAT 143:26622

AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.

L90 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2004:514933 CAPLUS Full-text

DOCUMENT NUMBER: 141:174024

TITLE: Synthesis of benzo[b]naphtho[2,3-d]furan-6,11-dione via one-pot remote anionic Fries rearrangement and metalation reaction

AUTHOR(S): Azevedo, Mariangela S.; Alves, Glaucia B. C.; Cardoso, Jari N.; Lopes, Rosângela S. C.; Lopes, Claudio C.

CORPORATE SOURCE: Instituto de Química, Departamento de Química Orgânica, CT, Universidade Federal do Rio de Janeiro, Rio de Janeiro, 21949 900, Brazil

SOURCE: Synthesis (2004), (8), 1262-1268

CODEN: SYNTBF; ISSN: 0039-7881

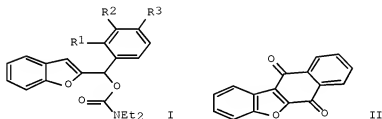
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:174024

GI



AB The use of a lithiation reaction to transform the arylcarbamate I (R1 = Br; R2= R3 = H) into the corresponding benzo[b]naphtho[2,3-d]furan-6,11-dione II is described. I (R1 = H; R2 = R3 = OMe; R2R3 = OCH2O) underwent the anionic Fried rearrangement, when reacted with s-butyllithium, to give the corresponding carboxamidoaryl carbinols.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:299566 CAPLUS Full-text

DOCUMENT NUMBER: 144:331264

10/595943

TITLE: Process for the preparation of substituted coumarin derivatives

INVENTOR(S): Carvalho, Jose Roque Mota; Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Slana, Glaucia Barbosa Alves; Guerra, Maicon

PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro - UFRJ, Brazil

SOURCE: PCT Int. Appl., 14 pp.

CODEN: PIXXD2

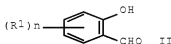
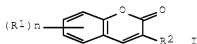
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006032120	A2	20060330	WO 2005-BR188	20050920
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW</p> <p>RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p>				
BR 2004004130	A	20060502	BR 2004-4130	20040920
US 20080011985	A1	20080117	US 2007-574845	20070307
PRIORITY APPLN. INFO.:			BR 2004-4130	A 20040920
			WO 2005-BR188	W 20050920
OTHER SOURCE(S):		MARPAT 144:331264		
GI				



AB A process for the preparation of coumarin derivs., such as I [R₁ = OH, CN, alkyl, alkenyl, alkynyl, aryl, acyl, halogen, dialkylamino, etc.; R₂ = alkyl, alkenyl, alkynyl, etc.; n = 1, 2, 3, or 4], via cyclocondensation of corresponding 2-hydroxybenzaldehyde derivs. II with carboxylic acids R₂CO₂H. These coumarin derivs. are fluorescent when irradiated by UV light.

L90 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

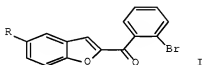
ACCESSION NUMBER: 2006:1289630 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:406621

TITLE: A novel synthesis of α-bromoacetophenones and its application in obtaining 2-benzoylbenzofurans

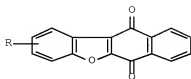
AUTHOR(S): Azevedo, Mariangela S.; Alves, Ana Paula L.; Alves,

Glauca B. C.; Cardoso, Jari N.; Lopes, Rosângela
 S. C.; Lopes, Claudio C.
 CORPORATE SOURCE: Departamento de Química Analítica, Instituto de
 Química, Universidade Federal do Rio de Janeiro, Rio
 de Janeiro, 21949-900, Brazil
 SOURCE: Química Nova (2006), 29(6), 1259-1265
 CODEN: QUNODK; ISSN: 0100-4042
 PUBLISHER: Sociedade Brasileira de Química
 DOCUMENT TYPE: Journal
 LANGUAGE: Portuguese
 OTHER SOURCE(S): CASREACT 147:406621
 GI

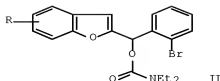


AB α -Bromoacetophenones are important in organic synthesis. They have been
 widely used as precursors of several natural products. Several methods of
 their synthesis via bromination have been described, however they furnish a
 mixture of starting material, mono and dibromide products. A novel, simple
 and efficient synthesis of these compds. have been developed and further
 applied to the preparation of benzoylbenzofurans, e.g., I (R = H or MeO).
 Benzoylbenzofurans are compds. with important pharmacol. properties, such as
 the ability of dilating the coronary artery and analgesic action. Such
 compds. have also been used as key intermediates to obtain quinone systems.
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 2006:301972 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 146:316668
 TITLE: Total syntheses of oxygenated brazanquinones via
 regioselective homologous anionic Fries rearrangement
 of benzylic O-carbamates
 AUTHOR(S): Slana, Glauca G. B. C. A. S.; Azevedo, Mariângela M.
 S. A.; Cardoso, Jari J. N. C.; Lopes, Rosângela R.
 S. C. L.; Lopes, Claudio C. C. L.
 CORPORATE SOURCE: Instituto de Química, Universidade Federal do Rio de
 Janeiro, Rio de Janeiro, 21949-900, Brazil
 SOURCE: Beilstein Journal of Organic Chemistry (2006),
 2(Feb.), No pp. given
 CODEN: BJOCBH; ISSN: 1860-5397
 URL: [http://bjoc.beilstein-](http://bjoc.beilstein-journals.org/content/pdf/1860-5397-2-1.pdf)
[journals.org/content/pdf/1860-5397-2-1.pdf](http://bjoc.beilstein-journals.org/content/pdf/1860-5397-2-1.pdf)
 PUBLISHER: Beilstein-Institut zur Foerderung der Chemischen
 Wissenschaften
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 GI



I



II

AB Using new variations of anionic aromatic chemical, the total synthesis of oxygenated brazanquinones I [R = 8-OMe, 7-OMe, 6-OMe], derived from β -brasan, a natural product isolated from *Caesalpinia echinata*, via carbamates II is described.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2006:1357896 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 146:45735

TITLE: Process for the preparation of aspartame derivative

INVENTOR(S): Costa da Silva, Jaciara; Lopes, Claudio Carqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Albert, Andre Luis Mazzei

PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro - Ufrj, Brazil

SOURCE: Braz. Pedido PI, 14pp.

CODEN: BPXXDX

DOCUMENT TYPE: Patent

LANGUAGE: Portuguese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BR 2004000467	A	20051116	BR 2004-467	20040308
PRIORITY APPLN. INFO.:			BR 2004-467	20040308
OTHER SOURCE(S):			CASREACT 146:45735; MARPAT 146:45735	

AB The invention relates to aspartame derivs. R²CC-L-Asp-L-Phe-OMe (R is C1-8 alkyl) or acceptable salts, which are sweet and have improved thermal stability. Thus, treatment of aspartame with (tert-butoxycarbonyloxyimino)phenylacetonitrile (Boc-ON) in aqueous dioxane in the presence of triethylamine afforded Boc-aspartame.

L90 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2003:52767 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:358454

TITLE: Pyrazolinone-piperidine dipeptide growth hormone

AUTHOR(S): secretagogues (GHSs): discovery of capromorelin
Carpino, Philip A.; Lefker, Bruce A.; Toler, Steven M.; Pan, Lydia C.; Hadcock, John R.; Cook, Ewell R.; DiBrino, Joseph N.; Campeta, Anthony M.; DeNinno, Shari L.; Chidsey-Frink, Kristin L.; Hada, William A.; Inthavongsay, John; Mangano, F. Michael; Mullins, Michelle A.; Nickerson, David F.; Ng, Oicheng; Pirie, Christine M.; Ragan, John A.; Rose, Colin R.; Tess, David A.; Wright, Ann S.; Yu, Li; Zawistoski, Michael P.; DaSilva-Jardine, Paul A.; Wilson, Theresa C.;

Thompson, David D.
 GROTON SOURCE: Groton Labs, Pfizer Global Research and Development,
 Groton, CT, 06340, USA
 SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(4),
 581-590
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:358454

AB Novel pyrazolinone-piperidine dipeptide derivs. were synthesized and evaluated as growth hormone secretagogues (GHSs). Two analogs, capromorelin (5, CP-424391-18, hGHS-R1a Ki=7 nM, rat pituitary EC50=3 nM) and the des-Me analog 5c (hGHS-R1a Ki=17 nM, rat pituitary EC50=3 nM), increased plasma GH levels in an anesthetized rat model, with ED50 values less than 0.05 mg/kg iv. Capromorelin showed enhanced intestinal absorption in rodent models and exhibited superior pharmacokinetic properties, including high bioavailabilities in two animal species [F(rat)=65%, F(dog)=44%]. This short-duration GHS was orally active in canine models and was selected as a development candidate for the treatment of musculoskeletal frailty in elderly adults.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 2002:808833 CAPLUS Full-text
 DOCUMENT NUMBER: 138:378539
 TITLE: Discovery and biological characterization of capromorelin analogues with extended half-lives
 AUTHOR(S): Carpino, Philip A.; Lefker, Bruce A.; Toler, Steven M.; Pan, Lydia C.; Haddock, John R.; Murray, Marianne C.; Cook, Ewell R.; Di Brino, Joseph N.; De Ninno, Shari L.; Chidsey-Frink, Kristin L.; Hada, William A.; Inthavongsay, John; Lewis, Sharon K.; Mangano, F. Michael; Mullins, Michelle A.; Nickerson, David F.; Ng, Oicheng; Pirie, Christine M.; Ragan, John A.; Rose, Colin R.; Tess, David A.; Wright, Ann S.; Yu, Li; Zawistoski, Michael P.; Pettersen, John C.; Da Silva-Jardine, Paul A.; Wilson, Theresa C.; Thompson, David D.

CORPORATE SOURCE: Groton Labs, Pfizer Global Research & Development,
 Groton, CT, 06340, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),
 12(22), 3279-3282
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:378539

AB New tert-Bu, picolyl and fluorinated analogs of capromorelin, a short-acting growth hormone secretagogue (GHS), were prepared as part of a program to identify long-acting GHSs that increase 24-h plasma IGF-1 levels. Some compds. (ACD LogD values ≥2.9) displayed extended plasma elimination half-lives in dogs, primarily due to high vols. of distribution, but showed weak GH secretagogue activities in rats (ED50s>10 mg/kg). A less lipophilic derivative CP-464709-18 (ACD LogD=1.6) exhibited a shorter canine half-life, but stimulated GH secretion in two animal species. Repeat oral dosing of CP-464709-18 to dogs for 29 days (6 mg/kg) resulted in a significant down-regulation of the post dose GH response and a 60 and 40% increase in IGF-1

levels relative to pre-dose levels at the 8- and 24-h post dose time points.
CP-464709-18 was selected as a candidate for the treatment of frailty.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:858884 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:169800

TITLE: Study of the protonation/deprotonation sequence of two
polyamines: bis-[(2S)-2-
pyrrolidinylmethyl]ethylenediamine and spermidine by
1H and 13C nuclear magnetic resonance

AUTHOR(S): Da Silva, Jacqueline Alves; Felcman, Judith; Lopes,
Claudio Cerqueira; Lopes, Rosangela S. C.; Villar,
Jose Daniel Figueroa

CORPORATE SOURCE: Department of Chemistry, Pontificia Universidade
Catolica do Rio de Janeiro, PUC, Rio de Janeiro,
Brazil

SOURCE: Spectroscopy Letters (2002), 35(5), 643-661

CODEN: SPLEBX; ISSN: 0038-7010

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:169800

AB In this paper we describe the study of protonation/deprotonation of two
polyamines: bis[(2S)-2-pyrrolidinylmethyl]ethylenediamine (tetra) and
spermidine (Spd). A new synthetic route was established for the synthesis of
tetra, which structure was confirmed by IR, elemental anal., 1H-NMR, 13C-
NMR(Pendant) and 2D-NMR (COSY, 13C-1H HETCOR and HMQC) spectra. The
protonation/deprotonation sequence studies of tetra and Spd were determined by
potentiometric and NMR methods. For the NMR studies, the tetra and Spd
samples were dissolved in D2O and the pD adjusted with NaOD. The
protonation/deprotonation sequences of tetra and Spd were determined by means
of the values and the variations of the hydrogen atom and 13C NMR chemical
shifts as a function of hydrogen atom pD. The variation of δ 1H with pD
clearly showed that the first protonation of tetra occurs at the pyrrolidine
nitrogen atoms and the second protonation occurs at the ethylenediamine
nitrogen atom. The anal. of the 13C-NMR spectra confirmed the results
obtained by 1H-NMR, as a greater chemical shift variation was observed for C-6
(5.6 ppm), as compared to C-8 (1.8 ppm). In the study with Spd, the greater
chemical shift variation was observed for C-2 (6.75 ppm) and C-5 (4.95 ppm),
indicating that the deprotonation occurs first at the secondary nitrogen atoms
and the second and third deprotonation steps occur at the primary nitrogen
atoms.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L90 ANSWER 11 OF 11 MEDLINE on STN

ACCESSION NUMBER: 2006162323 MEDLINE [Full-text](#)

DOCUMENT NUMBER: PubMed ID: 16542010

TITLE: Total syntheses of oxygenated brazanquinones via
regioselective homologous anionic Fries rearrangement of
benzylic O-carbamates.

AUTHOR: Slana Glauca Barbosa Candido Alves; de Azevedo Mariangela
Soares; Lopes Rosangela Sabattini Capella; Lopes Claudio
Cerqueira; Cardoso Jari Nobrega

CORPORATE SOURCE: Instituto de Quimica, Universidade Federal do Rio de

10/595943

Janeiro, CT, Bl A/508, 21949-900 Rio de Janeiro - RJ,
Brazil.. glaucia@gmx.net
SOURCE: Beilstein journal of organic chemistry, (2006) Vol. 2, No.
1, pp. 1. Electronic Publication: 2006-02-21.
Journal code: 101250746. E-ISSN: 1860-5397.
PUB. COUNTRY: Germany: Germany, Federal Republic of
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: NONMEDLINE; PUBMED-NOT-MEDLINE
ENTRY MONTH: 200604
ENTRY DATE: Entered STN: 23 Mar 2006
Last Updated on STN: 27 Apr 2006
Entered Medline: 26 Apr 2006

ABSTRACT:

Using new variations of anionic aromatic chemistry, the total synthesis of oxygenated brazanquinones (1a-1c), derived from beta-brasan, a natural product isolated from *Caesalpinia echinata*, via carbamates 2a-2c is described.

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 DICTIONARY FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5

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FILE CONTENT:1840 - 12 Oct 2008 VOL 149 ISS 16

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=> d stat que L43

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Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 (4732 REACTIONS)

L42 152 SEA FILE=CASREACT ABB=ON PLU=ON 10026-12-7

L43 1 SEA FILE=CASREACT ABB=ON PLU=ON L42 (L) L8

=> d ibib abs hit L43 1

L43 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 143:26622 CASREACT Full-text

TITLE: Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids
INVENTOR(S): Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Alves Da Silva, Jacqueline; Ferreira Gomes, Leticia

PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro-UFRJ, Brazil
SOURCE: PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

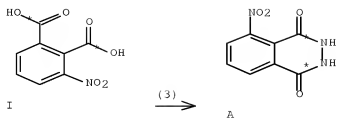
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051870	A2	20050609	WO 2004-BR236	20041125
WO 2005051870	A3	20050707		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
BR 2003007864	A	20050705	BR 2003-7864	20031125
US 20070128680	A1	20070607	US 2006-595943	20060522
PRIORITY APPLN. INFO.:			BR 2003-7864	20031125
			WO 2004-BR236	20041125

OTHER SOURCE(S): MARPAT 143:26622

AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.



RX(3) RCT I 603-11-0

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

SUBSTAGE(2) 4 hours, 50 deg C

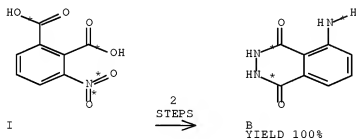
SUBSTAGE(3) cooled

PRO A 3682-15-3

NTE inert

RX(5) OF 6 COMPOSED OF RX(3), RX(1)

RX(5) I ==> E



RX(3) RCT I 603-11-0

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

10/595943

SUBSTAGE(2) 4 hours, 50 deg C
SUBSTAGE(3) cooled

PRO A 3682-15-3
NTE inert

RX(1) RCT A 3682-15-3
RGT C 1333-74-0 H2
PRO B 521-31-3
CAT 7440-05-3 Pd
SOL 123-91-1 Dioxane, 7732-18-5 Water, 64-19-7 AcOH
CON room temperature
NTE Pd supported on carbon was used as catalyst, sodium dithionite
in acidic medium can also be used as reducing agent

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REGISTRY includes numerically searchable data for experimental and
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FILE CONTENT:1840 - 12 Oct 2008 VOL 149 ISS 16

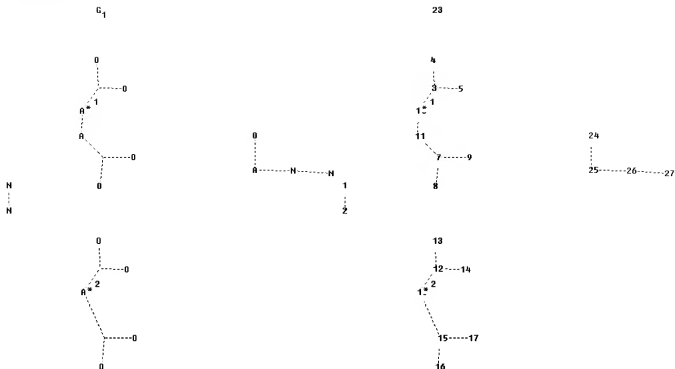
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```

chain nodes :
3 4 5 7 8 9 12 13 14 15 16 17 23 24
ring/chain nodes :
1 2 10 11 18 25 26 27
chain bonds :
3-4 3-5 3-10 7-8 7-9 7-11 12-13 12-14 12-18 15-16 15-17 15-18 24-25
ring/chain bonds :
1-2 10-11 25-26 26-27
exact/norm bonds :
1-2 3-4 3-5 3-10 7-8 7-9 7-11 10-11 12-13 12-14 12-18 15-16 15-17 15-18
24-25 25-26 26-27

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G1:[*1],[*2]

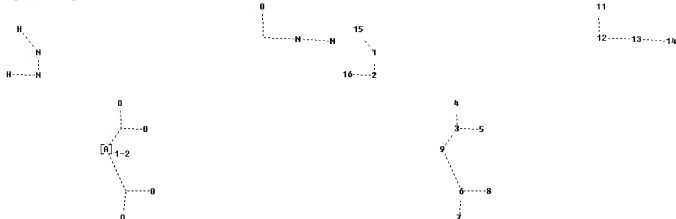
Connectivity :

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3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
7:3 E exact RC ring/chain 8:1 E exact RC ring/chain 9:1 E exact RC ring/chain
12:3 E exact RC ring/chain
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:3 E exact RC ring/chain
16:1
E exact RC ring/chain 17:1 E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS
fragments assigned product role:
containing 24
fragments assigned reactant/reagent role:
containing 1
containing 23

```

Uploading L59.str



```

chain nodes :
4 5 7 8 11 15 16
ring/chain nodes :
1 2 3 6 9 12 13 14
chain bonds :
1-15 2-16 3-4 3-5 6-7 6-8 11-12
ring/chain bonds :
1-2 3-9 6-9 12-13 13-14
exact/norm bonds :
1-2 1-15 2-16 3-4 3-5 3-9 6-7 6-8 6-9 11-12 12-13 13-14

```

```

Connectivity :
3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
6:3 E exact RC ring/chain 7:1 E exact RC ring/chain 8:1 E exact RC ring/chain
11:1 E exact RC ring/chain

```

```

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS
fragments assigned reactant role:
containing 3
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
reaction site bonds:
12-13:CC
node mappings:
3:12 1:13

```

```

=> d stat que L62
L6 STR

```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

10/595943

Structure attributes must be viewed using STN Express query preparation.
L8 446 SEA FILE=CASREACT SSS FUL L6 (4732 REACTIONS)
L20 2766 SEA FILE=CASREACT ABB=ON PLU=ON LEWIS ACID?/CW
L59 STR

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Structure attributes must be viewed using STN Express query preparation.
L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 (1426 REACTIONS)
L62 1 SEA FILE=CASREACT ABB=ON PLU=ON L61 AND L20

=> d stat que L63
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8 446 SEA FILE=CASREACT SSS FUL L6 (4732 REACTIONS)
L21 9688 SEA FILE=CASREACT ABB=ON PLU=ON LEWIS ACID?/BI,NTE
L59 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 (1426 REACTIONS)
L63 1 SEA FILE=CASREACT ABB=ON PLU=ON L61 AND L21

=> d stat que L64
L2 28 SEA FILE=REGISTRY ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/
BI OR 10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR
10026-12-7/BI OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/B
I OR 13450-90-3/BI OR 22441-45-8/BI OR 7446-70-0/BI OR
7447-39-4/BI OR 7487-94-7/BI OR 7550-45-0/BI OR 7637-07-2/BI
OR 7646-79-9/BI OR 7646-85-7/BI OR 7647-18-9/BI OR 7705-07-9/BI
OR 7705-08-0/BI OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/B
I OR 7786-30-3/BI OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/
BI)
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8 446 SEA FILE=CASREACT SSS FUL L6 (4732 REACTIONS)
L12 TRANSFER PLU=ON L8 1- RX : 5601 TERMS
L13 5601 SEA FILE=REGISTRY ABB=ON PLU=ON L12/RN
L14 11 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND L2
L15 348 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND (M/ELS OR B/ELS OR
AS/ELS OR TE/ELS OR AT/ELS)
L16 97 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND X/ELS
L17 86 SEA FILE=REGISTRY ABB=ON PLU=ON L16 NOT L14
L18 62 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND C/ELS
L19 24 SEA FILE=REGISTRY ABB=ON PLU=ON L17 NOT L18
L29 35 SEA FILE=REGISTRY ABB=ON PLU=ON L14 OR L19
L30 106670 SEA FILE=CASREACT ABB=ON PLU=ON L29
L59 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

10/595943

Structure attributes must be viewed using STN Express query preparation.

L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 (1426 REACTIONS)
L64 30 SEA FILE=CASREACT ABB=ON PLU=ON L61 (L) L30

=> d stat que L65

L2 28 SEA FILE=REGISTRY ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/
BI OR 10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR
10026-12-7/BI OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/B
I OR 13450-90-3/BI OR 22441-45-8/BI OR 7446-70-0/BI OR
7447-39-4/BI OR 7487-94-7/BI OR 7550-45-0/BI OR 7637-07-2/BI
OR 7646-79-9/BI OR 7646-85-7/BI OR 7647-18-9/BI OR 7705-07-9/BI
OR 7705-08-0/BI OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/B
I OR 7786-30-3/BI OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/
BI)
STR

L6

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L8 446 SEA FILE=CASREACT SSS FUL L6 (4732 REACTIONS)
L12 TRANSFER PLU=ON L8 1- RX : 5601 TERMS
L13 5601 SEA FILE=REGISTRY ABB=ON PLU=ON L12/RN
L14 11 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND L2
L15 348 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND (M/ELS OR B/ELS OR
AS/ELS OR TE/ELS OR AT/ELS)
L16 97 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND X/ELS
L17 86 SEA FILE=REGISTRY ABB=ON PLU=ON L16 NOT L14
L18 62 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND C/ELS
L31 15382 SEA FILE=CASREACT ABB=ON PLU=ON L18/CAT
L59 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L61 163 SEA FILE=CASREACT SUB=L8 SSS FUL L59 (1426 REACTIONS)
L65 2 SEA FILE=CASREACT ABB=ON PLU=ON L61 (L) L31

=> s L62 or L63 or L64 or L65

L91 30 L62 OR L63 OR L64 OR L65

=> d ibib abs hit L91 1-30

L91 ANSWER 1 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 148:168645 CASREACT Full-text

TITLE: Iptycene-Derived Pyridazines and Phthalazines

AUTHOR(S): Bouffard, Jean; Eaton, Robert F.; Mueller, Peter;
Swager, Timothy M.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of
Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of Organic Chemistry (2007), 72(26),
10166-10180

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

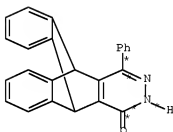
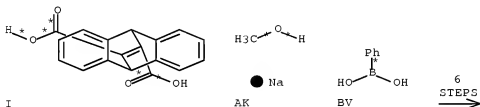
AB The synthesis of new heterocyclic oligo(phenylene) analogs based on soluble,
non-aggregating 1,2-diazines is reported. Improved palladium-catalyzed

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reductive coupling methods were developed to allow for the preparation of large quantities of iptycene-derived bipyridazine compds. and biphthalazine compds., and the controlled synthesis of well-defined oligomers up to sexipyridazine. Crystallog., spectroscopic, and computational evidence indicate that in these analogs, hindrance at the ortho position is relaxed relative to poly(phenylenes). The resulting building blocks are promising for incorporation in conjugated electronics materials and as new iptycene-derived ligands for transition metals.

REFERENCE COUNT: 113 THERE ARE 113 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

RX(279) OF 371 COMPOSED OF RX(7), RX(10), RX(13), RX(18), RX(41), RX(45)
RX(279) I + AK + BV ==> CR



CR
YIELD 72%

RX(7) RCT I 1625-61-6

STAGE(1)

CAT 68-12-2 DMF
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)

RGT Q 79-37-8 (COCl)2
CON overnight, 0 deg C -> room temperature

PRO P 1625-83-8

RX(10) RCT P 1625-83-8

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RGT W 2644-73-4 Hydrazine, hydrochloride (1:1)
 PRO V 937081-42-0
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) overnight, reflux
 SUBSTAGE(2) reflux -> room temperature

RX(13) RCT V 937081-42-0

STAGE(1)
 RGT AB 10025-87-3 POC13
 CON SUBSTAGE(1) overnight, reflux
 SUBSTAGE(2) reflux -> room temperature

STAGE(2)
 RGT AC 1344-28-1 Al2O3
 SOL 75-09-2 CH2Cl2
 CON 1 hour, room temperature

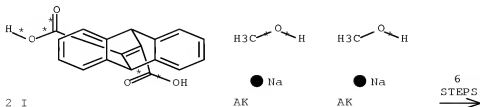
PRO AA 937081-43-1

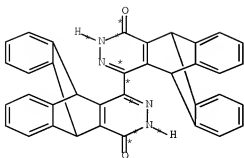
RX(18) RCT AA 937081-43-1, AK 124-41-4
 PRO AL 937081-49-7
 SOL 109-99-9 THF
 CON 22 hours, room temperature
 NTE chemoselective

RX(41) RCT AL 937081-49-7, BV 98-80-6
 RGT BS 13400-13-0 CsF
 PRO CK 937081-50-0
 CAT 14221-01-3 Pd(PPh3)4
 SOL 123-91-1 Dioxane
 CON SUBSTAGE(1) 48 hours, 115 deg C
 SUBSTAGE(2) 115 deg C -> room temperature
 NTE Suzuki coupling

RX(45) RCT CK 937081-50-0
 RGT CS 10035-10-6 HBr
 PRO CR 1001639-89-9
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) overnight, 90 deg C
 SUBSTAGE(2) 90 deg C -> room temperature
 NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

RX(281) OF 371 COMPOSED OF RX(7), RX(10), RX(13), RX(18), RX(50), RX(53)
 RX(281) 2 I + 2 AK ==> DH





DH
YIELD 91%

```

RX(7)      RCT   I 1625-81-6

            STAGE(1)
            CAT   68-12-2 DMF
            SOL   75-09-2 CH2Cl2
            CON   room temperature -> 0 deg C

            STAGE(2)
            RGT   Q 79-37-8 (COCl)2
            CON   overnight, 0 deg C -> room temperature

            PRO   P 1625-83-8

RX(10)     RCT   P 1625-83-8
            RGT   W 2644-70-4 Hydrazine, hydrochloride (1:1)
            PRO   V 937081-42-0
            SOL   64-19-7 AcOH
            CON   SUBSTAGE(1) overnight, reflux
                  SUBSTAGE(2) reflux -> room temperature

RX(13)     RCT   V 937081-42-0

            STAGE(1)
            RGT   AB 10025-87-3 POC13
            CON   SUBSTAGE(1) overnight, reflux
                  SUBSTAGE(2) reflux -> room temperature

            STAGE(2)
            RGT   AC 1344-28-1 Al2O3
            SOL   75-09-2 CH2Cl2
            CON   1 hour, room temperature

            PRO   AA 937081-43-1

RX(18)     RCT   AA 937081-43-1, AK 124-41-4
            PRO   AL 937081-49-7
            SOL   109-99-9 THF
            CON   22 hours, room temperature
            NTE   chemoselective

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RX(50) RCT AL 937081-49-7

STAGE(1)

RGT DA 7440-66-6 Zn

CAT 603-35-0 PPh3, 13965-03-2 PdCl2(PPh3)2

SOL 68-12-2 DMF

CON 20 hours, 100 deg C

STAGE(2)

RGT DB 139-33-3 Di-Na EDTA

SOL 7732-18-5 Water

PRO CZ 1001639-98-0

RX(53) RCT CZ 1001639-98-0

STAGE(1)

RGT CS 10035-10-6 HBr

SOL 64-19-7 AcOH

CON SUBSTAGE(1) overnight, 90 deg C

SUBSTAGE(2) 90 deg C -> room temperature

STAGE(2)

RGT CY 127-09-3 AcONa

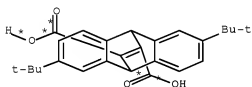
SOL 7732-18-5 Water

PRO DH 1001640-06-7

NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

RX(289) OF 371 COMPOSED OF RX(8), RX(11), RX(14), RX(19), RX(51), RX(54)

RX(289) 4 N + 4 AK ==> DI + DJ



4 N



● Na

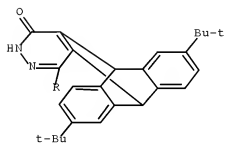
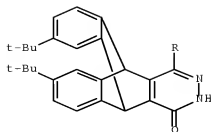
AK



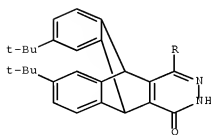
● Na

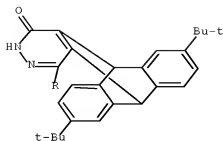
3 AK

6
STEPS
→



DI
YIELD 97% (50)





DJ
YIELD 97% (50)

RX(8) RCT N 1001639-36-6

STAGE(1)

CAT 68-12-2 DMF
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)

RGT Q 79-37-8 (COC1)2
CON overnight, 0 deg C -> room temperature

PRO T 1001639-38-8

RX(11) RCT T 1001639-38-8
RGT W 2644-70-4 Hydrazine, hydrochloride (1:1)
PRO Y 1001639-41-3
SOL 64-19-7 AcOH
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

RX(14) RCT Y 1001639-41-3

STAGE(1)

RGT AB 10025-87-3 POC13
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RGT AC 1344-28-1 Al2O3
SOL 75-09-2 CH2Cl2
CON 1 hour, room temperature

PRO AD 1001639-46-8

RX(19) RCT AD 1001639-46-8, AK 124-41-4
PRO AN 1001639-50-4
SOL 109-99-9 THF
CON 48 hours, room temperature
NTE chemoselective, reaction must be monitored by TLC to minimize formation of dimethoxy-substituted product or the isolation of unreacted starting material

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RX(51) RCT AN 1001639-50-4

STAGE(1)

RGT DA 7440-66-6 Zn
CAT 603-35-0 PPh₃, 13965-03-2 PdCl₂(PPh₃)₂
SOL 68-12-2 DMF
CON 20 hours, 100 deg C

STAGE(2)

RGT DB 139-33-3 Di-Na EDTA
SOL 7732-18-5 Water
CON 1 hour, room temperature

PRO DE 1001898-97-0, DF 1001899-70-2

RX(54) RCT DE 1001898-97-0, DF 1001899-70-2

STAGE(1)

RGT CS 10035-10-6 HBr
SOL 64-19-7 AcOH
CON SUBSTAGE(1) overnight, 95 deg C
SUBSTAGE(2) 95 deg C -> room temperature

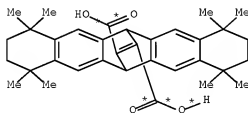
STAGE(2)

RGT CY 127-09-3 AcONa
SOL 7732-18-5 Water

PRO DI 1001898-98-1, DJ 1001899-01-9

NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

RX(293) OF 371 COMPOSED OF RX(9), RX(12), RX(15), RX(20), RX(52), RX(55)
RX(293) 2 O + 2 AK ==> DK



2 O



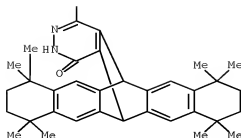
AK



AK

6
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



DK
YIELD 100%

RX(9) RCT O 1001639-37-7

STAGE(1)

CAT 68-12-2 DMF
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)

RGT Q 79-37-8 (COCl)₂
CON overnight, 0 deg C -> room temperature

PRO U 1001639-39-9

RX(12) RCT U 1001639-39-9
RGT W 2644-70-4 Hydrazine, hydrochloride (1:1)
PRO Z 1001639-43-5
SOL 64-19-7 AcOH
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

RX(15) RCT Z 1001639-43-5

STAGE(1)

RGT AB 10025-87-3 POC13
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RGT AC 1344-28-1 Al₂O₃
SOL 75-09-2 CH2Cl2
CON 1 hour, room temperature

PRO AE 1001639-47-9

RX(20) RCT AE 1001639-47-9, AK 124-41-4
PRO AO 1001639-52-6
SOL 109-99-9 THF
CON overnight, room temperature
NTE chemoselective, reaction must be monitored by TLC to minimize formation of dimethoxy-substituted product or the isolation of unreacted starting material

RX(52) RCT AO 1001639-52-6

STAGE(1)

RGT DA 7440-66-6 Zn
 CAT 603-35-0 PPh3, 13965-03-2 PdCl2(PPh3)2
 SOL 68-12-2 DMF
 CON 40 hours, 100 deg C

STAGE(2)

RGT DB 139-33-3 Di-Na EDTA
 SOL 7732-18-5 Water
 CON 1 hour

PRO DG 1001640-05-6

RX(55) RCT DG 1001640-05-6

STAGE(1)

RGT CS 10035-10-6 HBr
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) overnight, 95 deg C
 SUBSTAGE(2) 95 deg C -> room temperature

STAGE(2)

RGT CY 127-09-3 AcONa
 SOL 7732-18-5 Water

PRO DK 1001640-10-3

NTE violent release of gases (HBr, MeBr) occurs on warming the reaction, safety

L91 ANSWER 2 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:505354 CASREACT [Full-text](#)

TITLE: Synthesis and antimicrobial activity of succinimido (2-aryl-4-oxo-3-[[quinolin-8-yloxy]acetyl]amino)-1,3-thiazolidin-5-yl)acetates

AUTHOR(S): Ahmed, Maqbool; Sharma, Ranjana; Nagda, Devendra P.; Jat, Jawahar L.; Talesara, Ganpat L.

CORPORATE SOURCE: Synthetic Organic Chemistry Laboratory, Department of Chemistry, M. L. Sukhadia University, Udaipur, 313 001, India

SOURCE: ARKIVOC (Gainesville, FL, United States) (2006), (11), 66-75

CODEN: AGFUAR

URL: [http://www.arkat-](http://www.arkat-usa.org/ark/journal/2006/I11_General/1813/06-1813BP%20as%20published%20mainmanuscript.pdf)

[usa.org/ark/journal/2006/I11_General/1813/06-1813BP%20as%20published%20mainmanuscript.pdf](http://www.arkat-usa.org/ark/journal/2006/I11_General/1813/06-1813BP%20as%20published%20mainmanuscript.pdf)

Arkato USA Inc.

PUBLISHER: Journal; (online computer file)

DOCUMENT TYPE: English

LANGUAGE: English
 AB 8-Hydroxyquinoline reacts with ClCH2CO2Et in the presence of anhydrous K2CO3 to produce (quinolin-8-yloxy)acetate. Subsequent treatment with N2H4.H2O forms (quinolin-8-yloxy)acetyl hydrazide, which on condensation with aromatic aldehydes gives (quinolin-8-yloxy)acetyl (1Z)-arylidenehydrazides. The latter, on cyclization with mercaptosuccinate, yield (2-aryl-4-oxo-3-[[quinolin-8-yloxy]acetyl]amino)-1,3-thiazolidin-5-yl)acetates. Further conversion into acid chlorides and reaction with N-hydroxysuccinimide in the presence of TEA furnishes the title compds. Antibacterial and antifungal

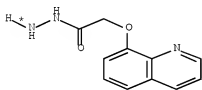
10/595943

activities of the final compds. were evaluated, and all the compds. inhibited bacterial and fungal growth.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(25) OF 69 COMPOSED OF RX(3), RX(8)

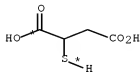
RX(25) F + I + T ==> U



F

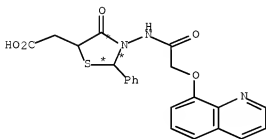


I



T

2
STEPS
→



U

YIELD 54%

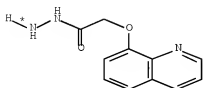
RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5
PRO U 914931-89-8
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

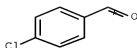
10/595943

RX(26) OF 69 COMPOSED OF RX(4), RX(9)

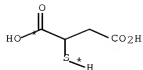
RX(26) F + L + T ==> X



F



L



T

2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT F 3281-08-1, L 104-88-1

PRO M 175688-48-9

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5

PRO X 914931-91-2

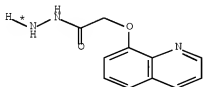
CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

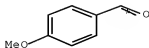
CON 12 - 14 hours, reflux

RX(27) OF 69 COMPOSED OF RX(5), RX(10)

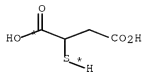
RX(27) F + N + T ==> Y



F



N



T

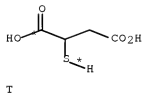
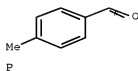
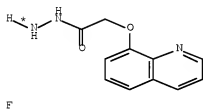
2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 3281-08-1, N 123-11-5
 PRO O 59836-00-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T 70-49-5
 PRO Y 914931-92-3
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(28) OF 69 COMPOSED OF RX(6), RX(11)
 RX(28) F + P + T ==> Z

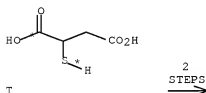
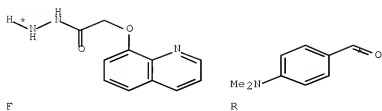


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(6) RCT F 3281-08-1, P 104-87-0
 PRO Q 358676-23-0
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5
 PRO Z 914931-93-4
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(29) OF 69 COMPOSED OF RX(7), RX(12)
 RX(29) F + R + T ==> AA

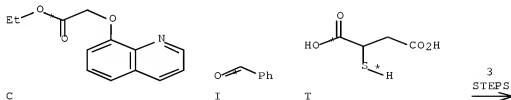


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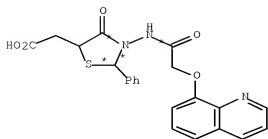
RX(7) RCT F 3281-03-1, R 100-10-7
 PRO S 59836-06-5
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-49-5
 PRO AA 914931-94-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(41) OF 69 COMPOSED OF RX(2), RX(3), RX(8)
 RX(41) C + I + T ==> U



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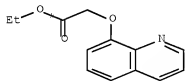
U
YIELD 54%

RX(2) RCT C 42322-30-5
RGT G 7803-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

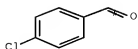
RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5
PRO U 914931-89-8
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

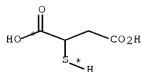
RX(42) OF 69 COMPOSED OF RX(2), RX(4), RX(9)
RX(42) C + L + T ==> X



C



L



T

3
STEPS
→

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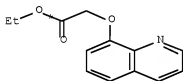
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 42322-30-5
 RGT G 7883-57-8 N2H4-H2O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

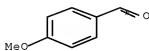
RX(4) RCT F 3281-08-1, L 104-88-1
 PRO M 175688-48-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 78-49-5
 PRO X 514931-91-2
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

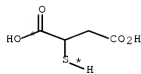
RX(43) OF 69 COMPOSED OF RX(2), RX(5), RX(10)
 RX(43) C + N + T ==> Y



C



N



T

3
 STEPS
 →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

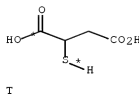
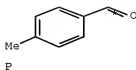
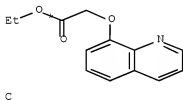
RX(2) RCT C 42322-30-5
 RGT G 7883-57-8 N2H4-H2O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(5) RCT F 3281-08-1, N 123-11-5
 PRO O 59836-00-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

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RX(10) RCT O 59836-00-9, T 70-49-5
 PRO Y 914931-92-3
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(44) OF 69 COMPOSED OF RX(2), RX(6), RX(11)
 RX(44) C + P + T ==> Z



3
 STEPS
 →

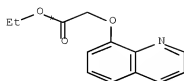
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 42322-30-5
 RGT G 7803-57-8 N2H4-H2O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

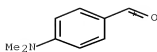
RX(6) RCT F 3281-08-1, P 104-87-0
 PRO Q 358676-23-0
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5
 PRO Z 914931-93-4
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

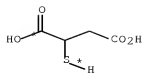
RX(45) OF 69 COMPOSED OF RX(2), RX(7), RX(12)
 RX(45) C + R + T ==> AA



C



R



T

3
STEPS
→

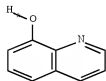
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 42322-30-5
RGT G 7603-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

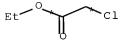
RX(7) RCT F 3281-08-1, R 100-10-7
PRO S 59836-06-5
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-43-5
PRO AA 914931-94-5
CAT 7646-95-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(46) OF 69 COMPOSED OF RX(1), RX(2), RX(3), RX(8)
RX(46) A + B + I + T ==> U



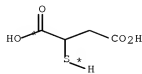
A



B

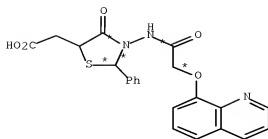


I



T

4
STEPS
→



U
YIELD 54%

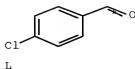
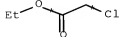
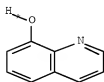
RX(1) RCT A 148-24-3, B 105-39-5
RGT D 584-08-7 K2CO3
PRO C 42322-30-5
SOL 67-64-1 Me2CO
CON 18 hours, reflux

RX(2) RCT C 42322-30-5
RGT G 7603-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

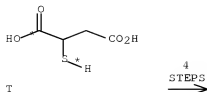
RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5
PRO U 914931-89-8
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(47) OF 69 COMPOSED OF RX(1), RX(2), RX(4), RX(9)
RX(47) A + B + L + T ==> X



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

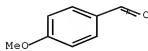
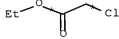
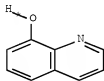
RX(1) RCT A 148-24-3, B 105-39-5
 RGT D 584-08-7 K₂CO₃
 PRO C 42322-30-5
 SOL 67-64-1 Me₂CO
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5
 RGT G 7803-57-8 N₂H₄-H₂O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

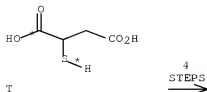
RX(4) RCT F 3281-08-1, L 104-88-1
 PRO M 175688-48-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5
 PRO X 914931-91-2
 CAT 7646-85-7 ZnCl₂
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(48) OF 69 COMPOSED OF RX(1), RX(2), RX(5), RX(10)
 RX(48) A + B + N + T ==> Y



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

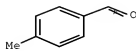
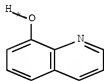
RX(1) RCT A 148-24-3, B 105-39-5
RGT D 584-08-7 K2CO3
PRO C 42322-30-5
SOL 67-64-1 Me2CO
CON 18 hours, reflux

RX(2) RCT C 42322-30-5
RGT G 7803-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

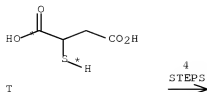
RX(5) RCT F 3281-08-1, N 123-11-5
PRO O 59836-00-9
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T 70-49-5
PRO Y 914931-92-3
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(49) OF 69 COMPOSED OF RX(1), RX(2), RX(6), RX(11)
RX(49) A + B + P + T ==> Z



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

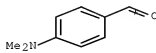
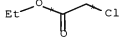
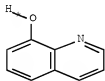
RX(1) RCT A 148-24-3, B 105-39-5
 RGT D 584-08-7 K₂CO₃
 PRO C 42322-30-5
 SOL 67-64-1 Me₂CO
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5
 RGT G 7803-57-8 N₂H₄·H₂O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

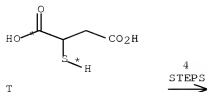
RX(6) RCT F 3281-08-1, P 104-87-0
 PRO Q 358676-23-0
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5
 PRO Z 914931-93-4
 CAT 7646-85-7 ZnCl₂
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(50) OF 69 COMPOSED OF RX(1), RX(2), RX(7), RX(12)
 RX(50) A + B + R + T ==> AA



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

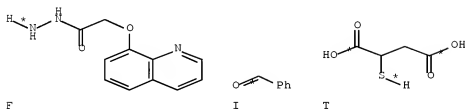
RX(1) RCT A 148-24-3, B 105-39-5
RGT D 584-08-7 K2CO3
PRO C 42322-30-5
SOL 67-64-1 Me2CO
CON 18 hours, reflux

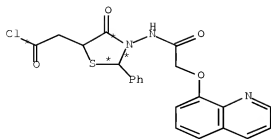
RX(2) RCT C 42322-30-5
RGT G 7803-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(7) RCT F 3281-08-1, R 100-10-7
PRO S 59836-06-5
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-49-5
PRO AA 914931-94-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(51) OF 69 COMPOSED OF RX(3), RX(8), RX(13)
RX(51) F + I + T ==> AB





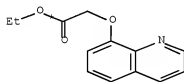
AB
YIELD 62%

RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5
PRO U 914931-89-8
CAT 7646-95-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8
RGT AC 7719-09-7 SOCl2
PRO AB 914931-95-6
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

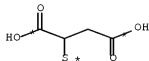
RX(52) OF 69 COMPOSED OF RX(2), RX(3), RX(8), RX(13)
RX(52) C + I + T ==> AB



C



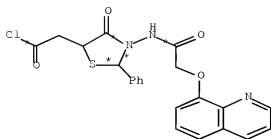
I



T

4
STEPS
→

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AB
YIELD 62%

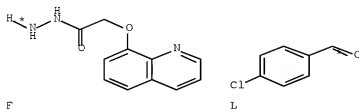
RX(2) RCT C 42322-30-5
RGT G 7803-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

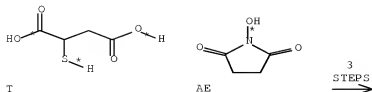
RX(8) RCT J 42322-33-8, I 70-49-5
PRO U 914931-89-8
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8
RGT AC 7719-09-7 SOCl2
PRO AB 914931-95-6
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

RX(53) OF 69 COMPOSED OF RX(4), RX(9), RX(15)
RX(53) F + L + T + AE ==> AI



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT F 3261-08-1, L 104-88-1
 PRO M 175688-48-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5
 PRO X 914931-91-2
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(15) RCT X 914931-91-2

STAGE(1)

 RGT AC 7719-09-7 SOCl2
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

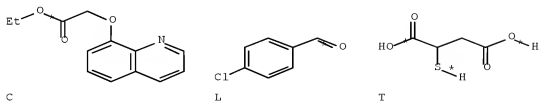
STAGE(2)

 RCT AE 6066-82-6
 RGT AG 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

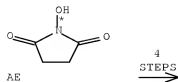
PRO AI 914931-97-9

RX(54) OF 69 COMPOSED OF RX(2), RX(4), RX(9), RX(15)

RX(54) C + L + T + AE ==> AI



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 42322-30-5
RGT G 7803-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(4) RCT F 3281-08-1, L 104-88-1
PRO M 175688-48-9
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5
PRO X 914931-91-2
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

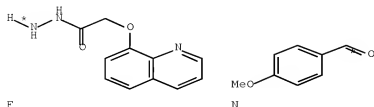
RX(15) RCT X 914931-91-2

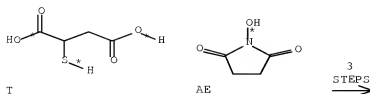
STAGE(1)
RGT AC 7719-09-7 SOCl2
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

STAGE(2)
RCT AE 6066-82-6
RGT AG 121-44-8 Et3N
SOL 68-12-2 DMF
CON 4 - 7 hours, reflux

PRO AI 914931-97-8

RX(55) OF 69 COMPOSED OF RX(5), RX(10), RX(16)
RX(55) F + N + T + AE ==> AJ





* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 3281-08-1, N 123-11-5
 PRO O 59836-00-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T 70-49-5
 PRO Y 914931-92-3
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(16) RCT Y 914931-92-3

STAGE(1)

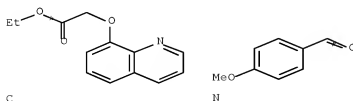
RGT AC 7719-09-7 SOCl2
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

STAGE(2)

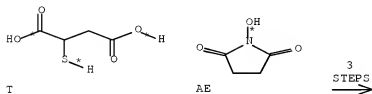
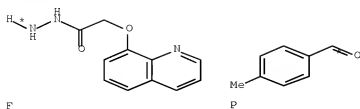
RCT AE 6066-82-6
 RGT AG 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

PRO AJ 914931-98-9

RX(56) OF 69 COMPOSED OF RX(2), RX(5), RX(10), RX(16)
 RX(56) C + N + T + AE ==> AJ



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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(6) RCT F 3281-06-1, P 104-87-0
 PRO Q 358676-23-0
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5
 PRO Z 914931-93-4
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(17) RCT Z 914931-93-4

STAGE(1)

RGT AC 7719-09-7 SOCl2
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

STAGE(2)

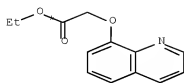
RCT AE 6066-82-6
 RGT AG 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

PRO AK 914931-99-0

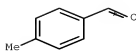
RX(58) OF 69 COMPOSED OF RX(2), RX(6), RX(11), RX(17)

RX(58) C + P + T + AE ==> AK

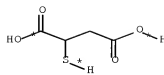
10/595943



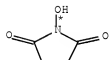
C



P



T



AE

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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RX(2)      RCT  C 42322-30-5
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 3281-08-1
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(6)      RCT  F 3281-08-1, P 104-87-0
           PRO  Q 358676-23-0
           CAT  64-19-7 AcOH
           SOL  64-17-5 EtOH
           CON  6 hours, reflux

RX(11)     RCT  Q 358676-23-0, T 70-49-5
           PRO  Z 914931-93-4
           CAT  7646-85-7 ZnCl2
           SOL  109-99-9 THF
           CON  12 - 14 hours, reflux

RX(17)     RCT  Z 914931-93-4

           STAGE(1)
           RGT  AC 7719-09-7 SOCl2
           SOL  71-43-2 Benzene
           CON  2 - 3 hours, reflux

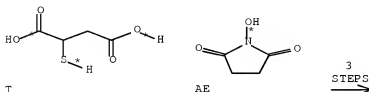
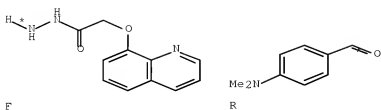
           STAGE(2)
           RCT  AE 6066-82-6
           RGT  AG 121-44-8 Et3N
           SOL  68-12-2 DMF
           CON  4 - 7 hours, reflux

PRO  AK 914931-99-0
  
```

RX(59) OF 69 COMPOSED OF RX(7), RX(12), RX(18)

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RX(59) F + R + T + AE ==> AL



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(7) RCT F 3281-08-1, R 100-10-7
 PRO S 59836-06-5
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-49-5
 PRO AA 914931-94-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(18) RCT AA 914931-94-5

STAGE(1)

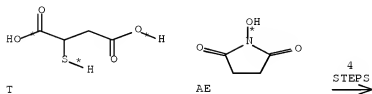
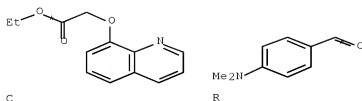
RGT AC 7719-09-7 SOCl2
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

STAGE(2)

RCT AE 6066-82-6
 RGT AG 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

PRO AL 914932-00-6

RX(60) OF 69 COMPOSED OF RX(2), RX(7), RX(12), RX(18)
 RX(60) C + R + T + AE ==> AL



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 42322-30-5
 RGT G 7893-57-8 N2H4-H2O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(7) RCT F 3281-08-1, R 100-10-7
 PRO S 59836-06-5
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(12) RCT S 59836-06-5, T 70-49-5
 PRO AA 914931-94-5
 CAT 7646-65-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(18) RCT AA 914931-94-5

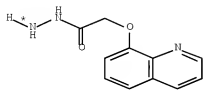
STAGE(1)
 RGT AC 7719-09-7 SOCl2
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

STAGE(2)
 RCT AE 6066-82-6
 RGT AG 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

PRO AL 914932-09-6

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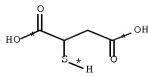
RX(62) OF 69 COMPOSED OF RX(3), RX(8), RX(13), RX(14)
 RX(62) F + I + T + AE ==> AF



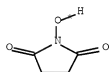
F



I

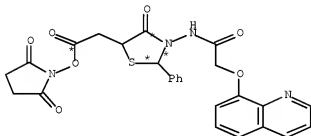


T



AE

4
STEPS
→



AF
YIELD 66%

RX(3) RCT F 3261-08-1, I 100-52-7
 PRO J 42322-33-8
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(8) RCT J 42322-33-8, T 70-49-5
 PRO U 914931-89-8
 CAT 7646-85-1 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

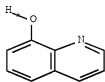
RX(13) RCT U 914931-89-8
 RGT AC 7719-09-7 SOCl2
 PRO AB 914931-95-6

10/595943

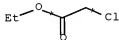
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

RX(14) RCT AB 914931-95-6, AE 6066-82-6
RGT AG 121-44-8 Et3N
PRO AF 914931-96-7
SOL 68-12-2 DMF
CON 4 - 7 hours, reflux

RX(63) OF 69 COMPOSED OF RX(1), RX(2), RX(3), RX(8), RX(13)
RX(63) A + B + I + T ==> AB



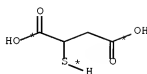
A



B

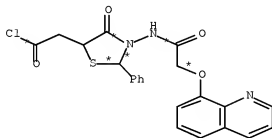


I



T

5
STEPS
→



AB
YIELD 62%

RX(1) RCT A 148-24-3, B 105-39-5
RGT D 584-08-7 K2CO3
PRO C 42322-30-5
SOL 67-64-1 Me2CO
CON 18 hours, reflux

RX(2) RCT C 42322-30-5
RGT G 7803-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

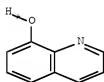
RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

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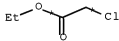
RX(8) RCT J 42322-33-8, T 70-49-5
 PRO U 914931-89-8
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8
 RGT AC 7719-09-7 SOCl2
 PRO AB 914931-95-6
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

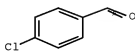
RX(64) OF 69 COMPOSED OF RX(1), RX(2), RX(4), RX(9), RX(15)
 RX(64) A + B + L + T + AE ==> AI



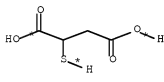
A



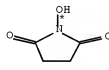
B



L



T



AE

5
 STEPS
 →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 148-24-3, B 105-39-5
 RGT D 584-08-7 K2CO3
 PRO C 42322-30-5
 SOL 67-64-1 Me2CO
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5
 RGT G 7803-57-8 N2H4-H2O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(4) RCT F 3281-08-1, L 104-88-1
 PRO M 175688-48-9
 CAT 64-19-7 AcOH

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SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(9) RCT M 175688-48-9, T 70-49-5
PRO X 914931-91-2
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

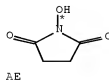
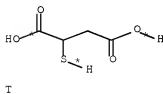
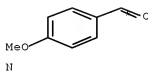
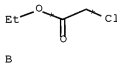
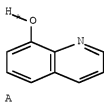
RX(15) RCT X 914931-91-2

STAGE(1)
RGT AC 7719-09-7 SOCl2
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

STAGE(2)
RCT AE 6066-82-6
RGT AG 121-44-8 Et3N
SOL 68-12-2 DMF
CON 4 - 7 hours, reflux

PRO AI 914931-97-8

RX(65) OF 69 COMPOSED OF RX(1), RX(2), RX(5), RX(10), RX(16)
RX(65) A + B + N + T + AE ==> AJ



5
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 148-24-3, B 105-39-5
RGT D 584-08-7 K2CO3
PRO C 42322-30-5
SOL 67-64-1 Me2CO

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CON 18 hours, reflux

RX(2) RCT C 42322-30-5
RGT G 7883-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(5) RCT F 3281-08-1, N 123-11-5
PRO O 59836-00-9
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(10) RCT O 59836-00-9, T 70-49-5
PRO Y 914931-92-3
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(16) RCT Y 914931-92-3

STAGE(1)

RGT AC 7719-09-7 SOCl2
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

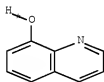
STAGE(2)

RCT AE 6066-82-6
RGT AG 121-44-8 Et3N
SOL 68-12-2 DMF
CON 4 - 7 hours, reflux

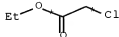
PRO AJ 914931-98-9

RX(66) OF 69 COMPOSED OF RX(1), RX(2), RX(6), RX(11), RX(17)

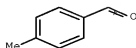
RX(66) A + B + P + T + AE ==> AK



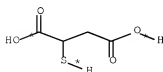
A



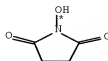
B



P



T



AE

5
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 148-24-3, B 105-39-5
 RGT D 584-08-7 K2CO3
 PRO C 42322-30-5
 SOL 67-64-1 Me2CO
 CON 18 hours, reflux

RX(2) RCT C 42322-30-5
 RGT G 7803-57-8 N2H4-H2O
 PRO F 3281-08-1
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(6) RCT F 3281-08-1, P 104-87-0
 PRO Q 358676-23-0
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 6 hours, reflux

RX(11) RCT Q 358676-23-0, T 70-49-5
 PRO Z 914931-93-4
 CAT 7646-95-7 ZnCl2
 SOL 109-99-9 THF
 CON 12 - 14 hours, reflux

RX(17) RCT Z 914931-93-4

STAGE(1)

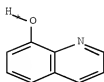
RGT AC 7719-09-7 SOCl2
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

STAGE(2)

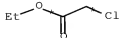
RCT AE 6066-82-6
 RGT AG 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

PRO AK 914931-99-0

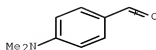
RX(67) OF 69 COMPOSED OF RX(1), RX(2), RX(7), RX(12), RX(18)
 RX(67) A + B + R + T + AE ==> AL



A

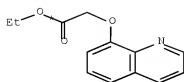


B



R

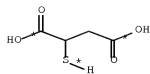
10/595943



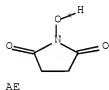
C



I

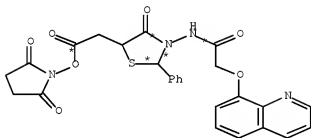


T



AE

5
STEPS
→



AF
YIELD 66%

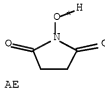
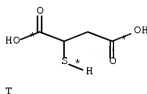
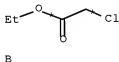
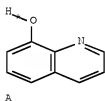
RX(2)	RCT	C 42322-30-5
	RGT	G 7803-57-8 N2H4-H2O
	PRO	F 3281-08-1
	SOL	64-17-5 EtOH
	CON	6 hours, reflux
RX(3)	RCT	F 3281-08-1, I 100-52-7
	PRO	J 42322-33-8
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	6 hours, reflux
RX(8)	RCT	J 42322-33-8, T 70-49-5
	PRO	U 914931-89-8
	CAT	7646-85-7 ZnCl2
	SOL	109-99-9 THF
	CON	12 - 14 hours, reflux

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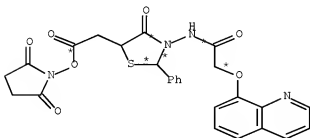
RX(13) RCT U 914931-89-8
 RGT AC 7719-09-7 SOC12
 PRO AB 914931-95-6
 SOL 71-43-2 Benzene
 CON 2 - 3 hours, reflux

RX(14) RCT AB 914931-95-6, AE 6066-82-6
 RGT AG 121-44-8 Et3N
 PRO AF 914931-96-7
 SOL 68-12-2 DMF
 CON 4 - 7 hours, reflux

RX(69) OF 69 COMPOSED OF RX(1), RX(2), RX(3), RX(8), RX(13), RX(14)
 RX(69) A + B + I + T + AE ==> AF



6
 STEPS
 ➔



AF
 YIELD 66%

RX(1) RCT A 148-24-3, B 105-39-5
 RGT D 584-08-7 K2CO3

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PRO C 42322-30-5
SOL 67-64-1 Me2CO
CON 18 hours, reflux

RX(2) RCT C 42322-30-5
RGT G 7893-57-8 N2H4-H2O
PRO F 3281-08-1
SOL 64-17-5 EtOH
CON 6 hours, reflux

RX(3) RCT F 3281-08-1, I 100-52-7
PRO J 42322-33-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 6 hours, reflux

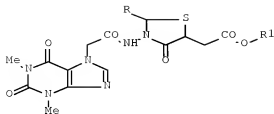
RX(8) RCT J 42322-33-8, T 78-49-5
PRO U 914931-89-8
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 12 - 14 hours, reflux

RX(13) RCT U 914931-89-8
RGT AC 7719-09-7 SOCl2
PRO AB 914931-95-6
SOL 71-43-2 Benzene
CON 2 - 3 hours, reflux

RX(14) RCT AB 914931-95-6, AE 6066-82-6
RGT AG 121-44-8 Et3N
PRO AF 914931-96-7
SOL 68-12-2 DMF
CON 4 - 7 hours, reflux

L91 ANSWER 3 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:188600 CASREACT Full-text
TITLE: Synthesis of phthalimido/succinimido [2-substituted
aryl-3-(N7-theophyllinylacetamidyl)-4-oxo-1,3-
thiazolidin-5-yl]ethanoic acids
AUTHOR(S): Sharma, Ranjana; Ahmed, Maqbool; Talesara, G. L.
CORPORATE SOURCE: Synthetic Organic Chemistry Laboratory, Department of
Chemistry, Mohan Lal Sukhadia University, Udaipur, 313
001, India
SOURCE: Indian Journal of Heterocyclic Chemistry (2005),
15(1), 35-38
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

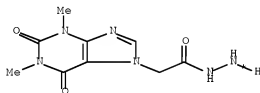


I

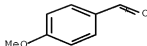
AB The title theophylline derivs. I [R = Ph, C₆H₄-4-OMe, -4-Cl, -3-NO₂, -4-NO₂, -4-NMe₂, C₆H₂-3,4,5-(OMe)₃, 2-furanyl; R₁ = phthalimido, succinimido] were prepared via reactions of Et N⁷-theophyllinyl acetate with hydrazine hydrate gives N⁷-theophyllinylacetyl hydrazide, which on condensation with various aromatic aldehydes, RCHO, afforded the corresponding arylidene derivs. A series of 2-substituted aryl-3-(N⁷-theophyllinylacetamidyl)-4-oxo-1,3-thiazolidin-5-yl ethanoic acids I (R₁ = H) were synthesized via cycloaddn. of the arylidene derivs. with mercaptosuccinic acid. The ethanoic acids were subsequently converted into the corresponding acid chlorides, which were in turn condensed with N-hydroxyphthalimide or N-hydroxysuccinimide to furnish title compds.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

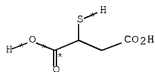
RX(3) OF 139 ...F + I + J ==> K...



F



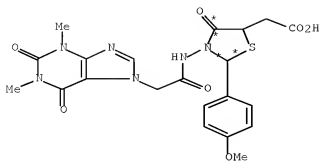
I



J



10/595943



K
YIELD 60%

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

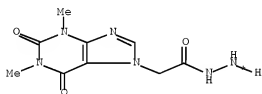
SOL 109-99-9 THF

CON 10 hours, reflux

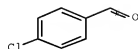
PRO K 901781-44-0

NTE intermediate was isolated

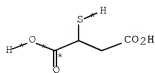
RX(21) OF 139 ...F + AS + J ==> AT...



F



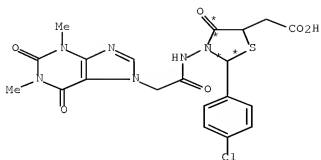
AS



J

(21)
→

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AT
YIELD 59%

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

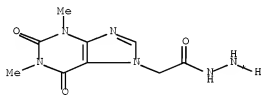
STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

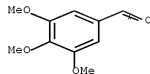
PRO AT 901781-62-2

NTE intermediate was isolated

RX(22) OF 139 ...F + AU + J ==> AV...

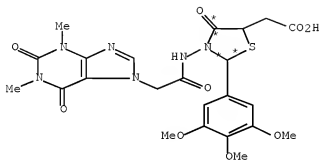
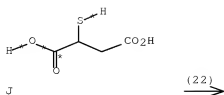


F



AU

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YIELD 63%

RX(22) RCT F 41638-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

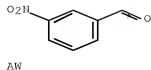
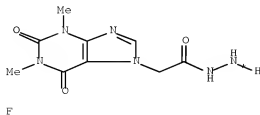
STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

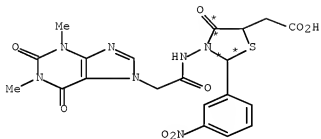
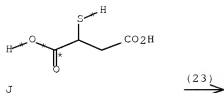
PRO AV 901781-63-3

NTE intermediate was isolated

RX(23) OF 139 ...F + AW + J ==> AX...



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AX
YIELD 67%

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

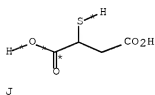
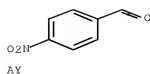
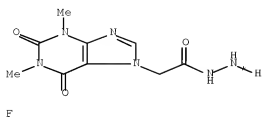
RCT J 70-49-5
CAT 7646-85-7 ZnCl₂
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AX 901781-64-4

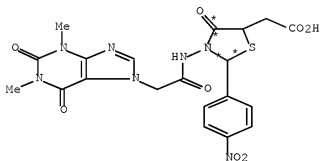
NTE intermediate was isolated

RX(24) OF 139 ...F + AY + J ==> AZ...

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(24) →



YIELD 61%

RX(24) RCT F 41638-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

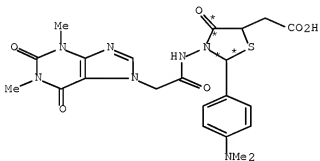
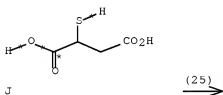
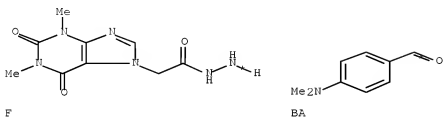
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AZ 901781-65-5

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NTE intermediate was isolated

RX(25) OF 139 ...F + BA + J ==> BB...



BB
YIELD 57%

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

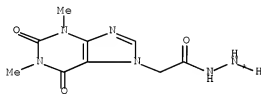
RCT J 70-49-5

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CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 561781-66-6
NTE intermediate was isolated

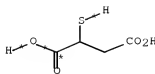
RX(26) OF 139 ...F + BC + J ==> BD...



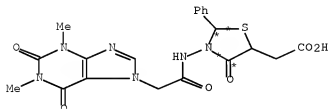
F



BC



J



BD
YIELD 70%

RX(26) RCT F 41836-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

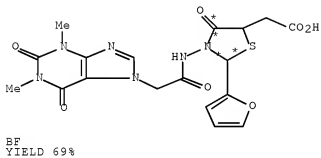
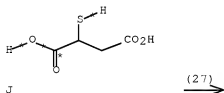
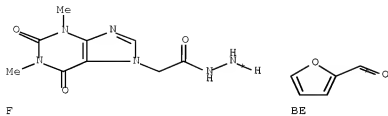
STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BD 561781-67-7
NTE intermediate was isolated

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RX(27) OF 139 ...F + BE + J ==> BF...



RX(27) RCT F 41838-05-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

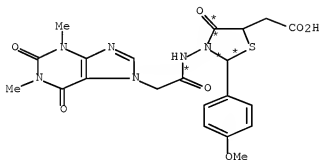
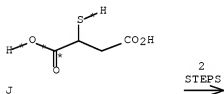
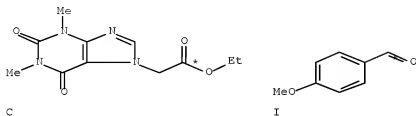
PRO BF 901781-68-8

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NTE intermediate was isolated

RX(36) OF 139 COMPOSED OF RX(2), RX(3)

RX(36) C + I + J ==> K



K
YIELD 60%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

10/595943

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

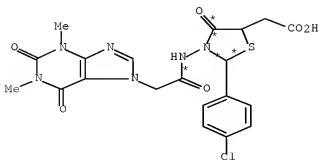
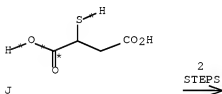
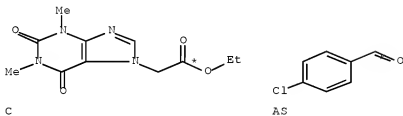
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO K 901781-44-0

NTE intermediate was isolated

RX(37) OF 139 COMPOSED OF RX(2), RX(21)

RX(37) C + AS + J ==> AT



AT
YIELD 59%

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RX(2) RCT C 7029-96-1
 RGT G 7883-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

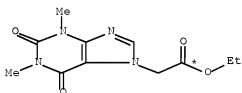
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AT 961781-62-2

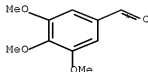
NTE intermediate was isolated

RX(38) OF 139 COMPOSED OF RX(2), RX(22)

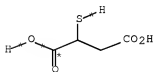
RX(38) C + AU + J ==> AV



C



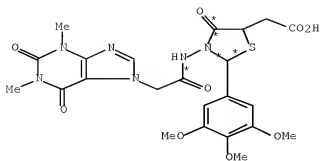
AU



J

2
STEPS
→

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AV
YIELD 63%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

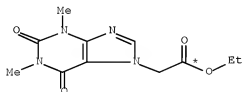
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AV 901781-63-3

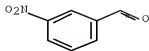
NTE intermediate was isolated

RX(39) OF 139 COMPOSED OF RX(2), RX(23)

RX(39) C + AW + J ==> AX

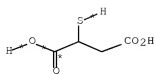


C



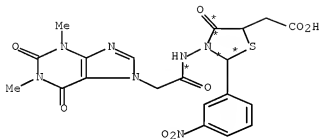
AW

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J

2
STEPS
→



AX

YIELD 67%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

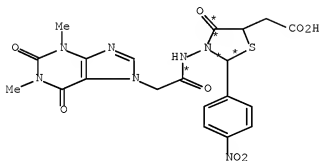
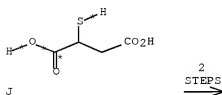
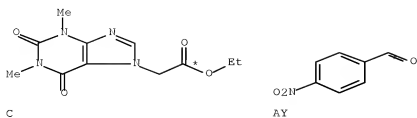
PRO AX 961781-64-4

NTE intermediate was isolated

RX(40) OF 139 COMPOSED OF RX(2), RX(24)

RX(40) C + AY + J ==> AZ

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RX(2) RCT C 7029-96-1
 RGT G 7603-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

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PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

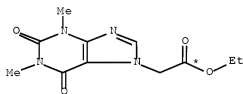
STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 901781-66-6
NTE intermediate was isolated

RX(42) OF 139 COMPOSED OF RX(2), RX(26)

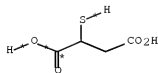
RX(42) C + BC + J ==> BD



C

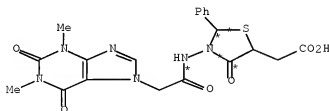


BC



J

2
STEPS
→



BD
YIELD 70%

RX(2) RCT C 7029-96-1
RGT G 7803-51-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

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STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

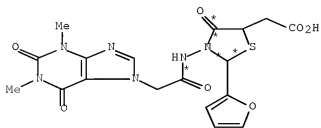
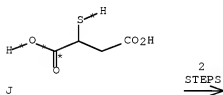
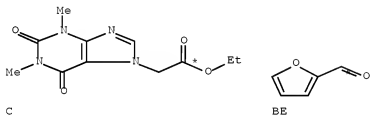
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BD 901791-67-7

NTE intermediate was isolated

RX(43) OF 139 COMPOSED OF RX(2), RX(27)

RX(43) C + BE + J ==> BF



YIELD 69%

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RX(2) RCT C 7029-96-1
 RGT G 7883-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

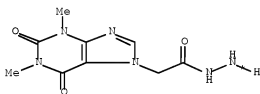
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO BF 961781-66-8

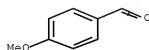
NTE intermediate was isolated

RX(44) OF 139 COMPOSED OF RX(3), RX(4)

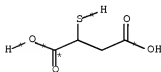
RX(44) F + I + J ==> F



F



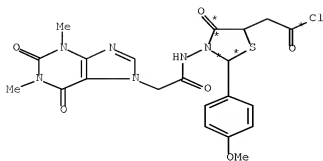
I



J

2
 STEPS
 →

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P
YIELD 43%

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

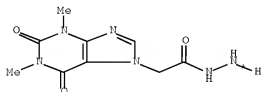
STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

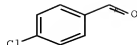
PRO K 901781-44-0
NTE intermediate was isolated

RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO F 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(47) OF 139 COMPOSED OF RX(21), RX(28)
RX(47) F + AS + J ==> V

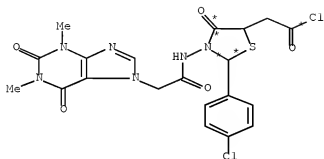
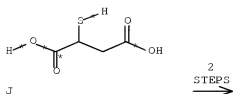


F



AS

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V
YIELD 52%

RX(21) RCT F 41638-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

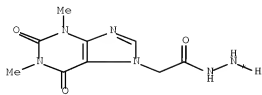
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AT 901781-62-2
NTE intermediate was isolated

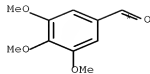
RX(28) RCT AT 901781-62-2
RGT Q 7719-09-7 SOCl2
PRO V 901781-62-2
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(48) OF 139 COMPOSED OF RX(22), RX(29)
RX(48) F + AU + J > X

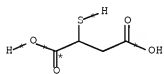
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F

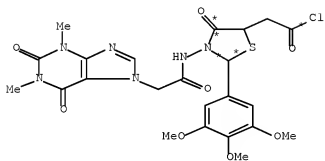


AU



J

2
STEPS
→



X

YIELD 47%

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 77-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AV 901781-63-3

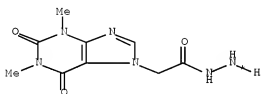
NTE intermediate was isolated

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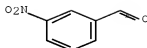
RX(29) RCT AV 901781-63-3
 RGT Q 7719-09-7 SOCl2
 PRO X 901781-70-2
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(49) OF 139 COMPOSED OF RX(23), RX(30)

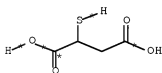
RX(49) F + AW + J ==> Z



F

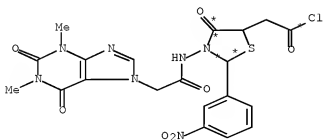


AW



J

2
STEPS
→



Z

YIELD 45%

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

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CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

PRO AX 901781-64-4

NTE intermediate was isolated

RX(30) RCT AX 901781-64-4

RGT Q 7719-09-7 SOCl2

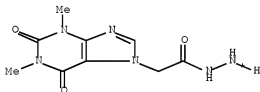
PRO Z 901781-71-3

SOL 108-88-3 PhMe

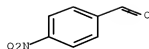
CON 30 minutes, reflux

RX(50) OF 139 COMPOSED OF RX(24), RX(31)

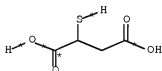
RX(50) F + AY + J ==> AB



F



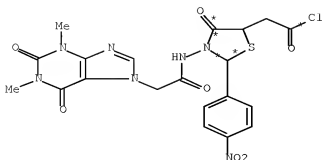
AY



J

2
STEPS
→

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AB
YIELD 55%

RX(24) RCT F 41638-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

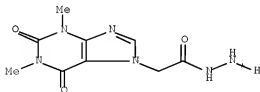
STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

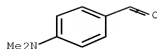
PRO AZ 901781-65-5
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOCl2
PRO AB 901781-72-4
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(51) OF 139 COMPOSED OF RX(25), RX(32)
RX(51) F + BA + J ==> AD

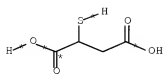


F



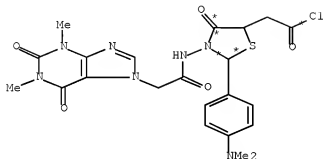
BA

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J

2
STEPS
→



AD
YIELD 60%

RX(25) RCT F 41836-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

PRO BB 901781-66-6

NTE intermediate was isolated

RX(32) RCT BB 901781-66-6

RGT Q 7719-09-7 SOCl2

PRO AD 901781-73-5

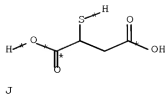
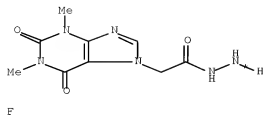
SOL 108-88-3 PhMe

CON 30 minutes, reflux

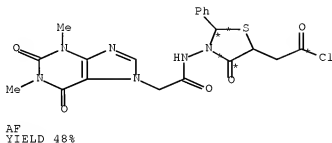
RX(52) OF 139 COMPOSED OF RX(26), RX(33)

RX(52) F + BC + J ==> PF

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2
STEPS
→



RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

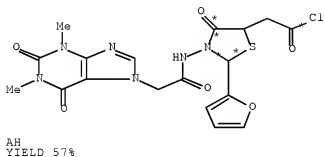
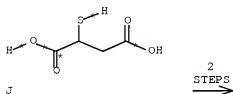
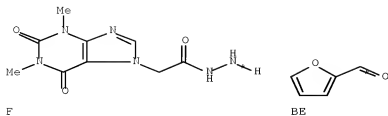
PRO BD 901781-67-7
NTE intermediate was isolated

RX(33) RCT BD 901781-67-7
RGT Q 7719-09-7 SOCl2
PRO AF 901781-74-6
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(53) OF 139 COMPOSED OF RX(27), RX(34)

RX(53) F + BE + J ==> AH

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RX(27) RCT F 41836-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BF 901781-68-8

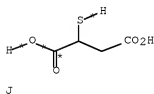
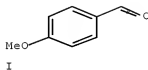
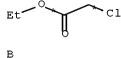
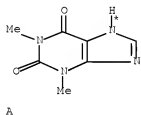
NTE intermediate was isolated

RX(34) RCT BF 901781-68-8

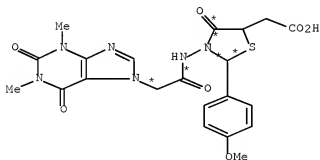
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RGT Q 7719-09-7 SOC12
 PRO AH 961781-75-7
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(68) OF 139 COMPOSED OF RX(1), RX(2), RX(3)
 RX(68) A + B + I + J ==> K



3
 STEPS
 →



K
 YIELD 60%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 2 hours, room temperature

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STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

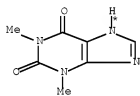
STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

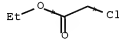
PRO K 901701-44-0
NTE intermediate was isolated

RX(69) OF 139 COMPOSED OF RX(1), RX(2), RX(21)

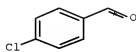
RX(69) A + B + AS + J ==> AT



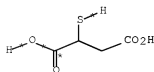
A



B



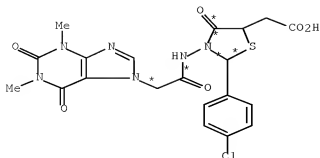
AS



J

3
STEPS
→

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AT
YIELD 59%

RX(1) RCT A 58-55-9
STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

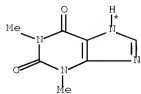
STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 78-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

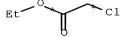
PRO AT 501781-62-2
NTE intermediate was isolated

RX(70) OF 139 COMPOSED OF RX(1), RX(2), RX(22)
RX(70) A + B + AU + J ==> AV

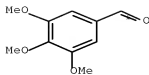
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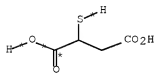
A



B

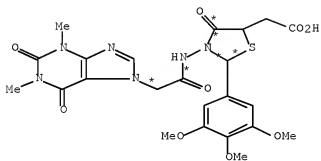


AU



J

3
STEPS
→



AV
YIELD 63%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

RGT G 7833-57-8 N2H4-H2O

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PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

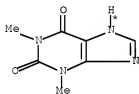
STAGE(2)

RCT J 70-49-5
CAT 7546-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

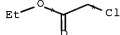
PRO AV 901781-63-3
NTE intermediate was isolated

RX(71) OF 139 COMPOSED OF RX(1), RX(2), RX(23)

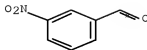
RX(71) A + B + AW + J ==> AX



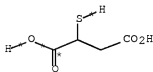
A



B



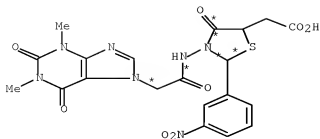
AW



J

3
STEPS
→

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AX
YIELD 67%

RX(1) RCT A 58-55-9

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

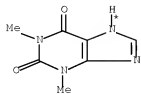
STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 70-49-5
CAT 7646-65-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

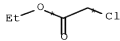
PRO AX 901781-64-4
NTE intermediate was isolated

RX(72) OF 139 COMPOSED OF RX(1), RX(2), RX(24)
RX(72) A + B + AY + J ==> AZ

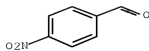
10/595943



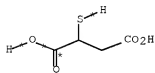
A



B

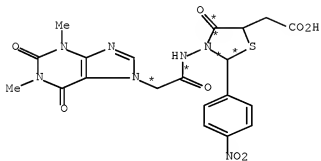


AY



J

3
STEPS
→



AZ
YIELD 61%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

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RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

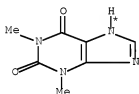
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AZ 901781-65-5

NTE intermediate was isolated

RX(73) OF 139 COMPOSED OF RX(1), RX(2), RX(25)

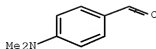
RX(73) A + B + BA + J ==> BB



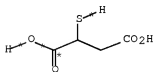
A



B



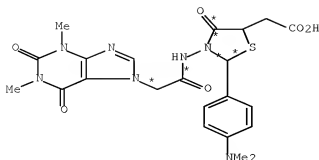
BA



J

3
STEPS
→

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BB
YIELD 57%

RX(1) RCT A 58-55-9
STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

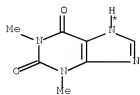
STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

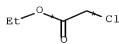
PRO BB 901781-66-6
NTE intermediate was isolated

RX(74) OF 139 COMPOSED OF RX(1), RX(2), RX(26)
RX(74) A + B + BC + J ==> ED

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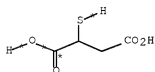
A



B

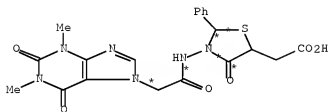


BC



J

3
STEPS
→



BD
YIELD 70%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2)

RCT C 7029-96-1

RGT G 7803-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

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RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

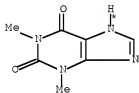
RCT J 73-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BD 901781-67-7

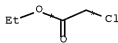
NTE intermediate was isolated

RX(75) OF 139 COMPOSED OF RX(1), RX(2), RX(27)

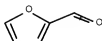
RX(75) A + B + BE + J ==> EF



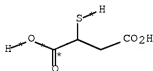
A



B



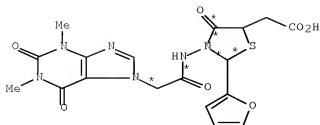
BE



J

3
STEPS
→

10/595943



BF
YIELD 69%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2)

RCT C 7029-96-1

RGT G 7663-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-43-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

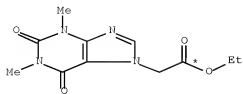
PRO BF 901781-68-8

NTE intermediate was isolated

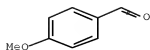
RX(76) OF 139 COMPOSED OF RX(2), RX(3), RX(4)

RX(76) C + I + J ==> F

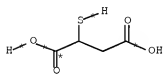
10/595943



C

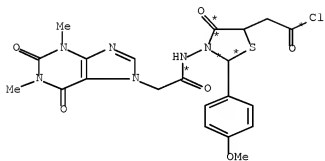


I



J

3
STEPS
→



P

YIELD 43%

RX(2) RCT C 7029-96-1
RGT G 7883-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

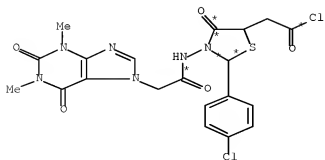
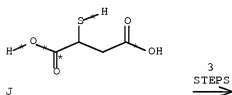
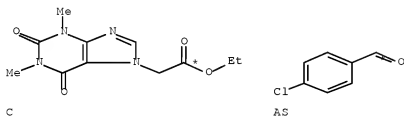
10/595943

CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO K 901781-44-0
NTE intermediate was isolated

RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(77) OF 139 COMPOSED OF RX(2), RX(21), RX(28)
RX(77) C + AS + J ==> V



YIELD 52%

RX(2) RCT C 7029-96-1
 RGT G 7883-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

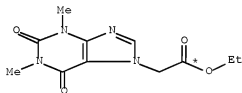
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AT 901781-62-2
 NIE intermediate was isolated

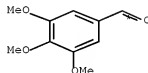
RX(28) RCT AT 901781-62-2
 RGT Q 7719-09-7 SOCl2
 PRO V 901781-62-2
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(78) OF 139 COMPOSED OF RX(2), RX(22), RX(29)

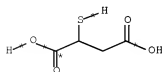
RX(78) C + AU + J ==> X



C

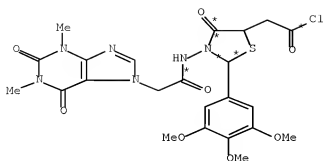


AU



J

3
 STEPS
 ➡



X
YIELD 47%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

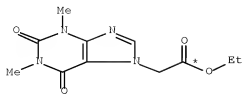
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AV 901781-63-3
NTE intermediate was isolated

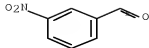
RX(29) RCT AV 901781-63-3
RGT Q 7719-09-7 SOCl2
PRO X 901781-70-2
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(79) OF 139 COMPOSED OF RX(2), RX(23), RX(30)
RX(79) C + AW + J ==> Z

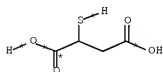
10/595943



C

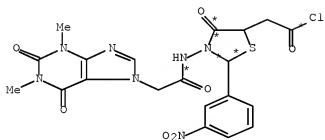


AW



J

3
STEPS
→



Z
YIELD 45%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 78-49-5
CAT 7646-85-7 ZnCl2

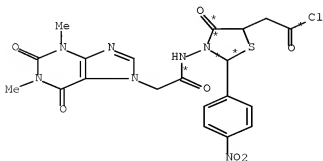
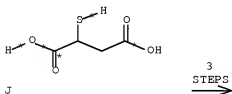
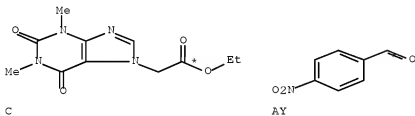
10/595943

SOL 109-99-9 THF
CON 10 hours, reflux

PRO AX 901781-64-4
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4
RGT Q 7719-09-7 SOCl₂
PRO Z 901761-71-3
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(80) OF 139 COMPOSED OF RX(2), RX(24), RX(31)
RX(80) C + AY + J ==> AB



YIELD 55%

RX(2) RCT C 7029-96-1
 RGT G 7883-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

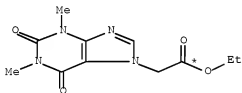
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AZ 901781-65-5
 NIE intermediate was isolated

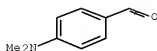
RX(31) RCT AZ 901781-65-5
 RGT Q 7719-09-7 SOCl2
 PRO AB 901781-72-4
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(81) OF 139 COMPOSED OF RX(2), RX(25), RX(32)

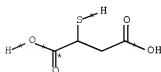
RX(81) C + BA + J ==> AD



C

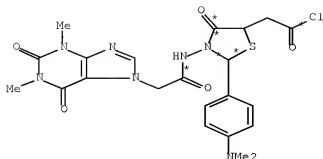


BA



J

3
 STEPS
 →



AD
YIELD 60%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

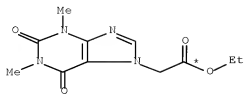
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 901781-66-6
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOCl2
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(82) OF 139 COMPOSED OF RX(2), RX(26), RX(33)
RX(82) C + BC + J ==> AF

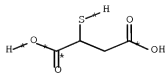
10/595943



C

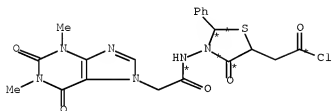


BC



J

3
STEPS
→



AF
YIELD 48%

RX(2) RCT C 7029-96-1
RGT G 7893-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 78-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

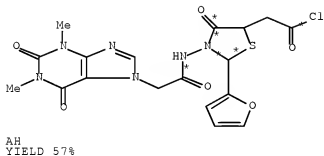
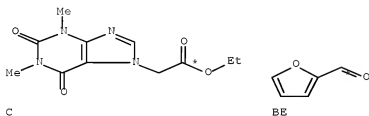
PRO BD 901781-67-7
NTE intermediate was isolated

RX(33) RCT BD 901781-67-7
RGT Q 7719-09-7 SOCl2

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PRO AF 901781-74-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(83) OF 139 COMPOSED OF RX(2), RX(27), RX(34)
RX(83) C + BE + J ==> AH



RX(2) RCT C 7029-96-1
RGT G 7893-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

10/595943

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

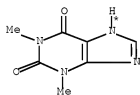
STAGE(2)

RCT J 770-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

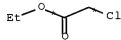
PRO BF 901781-68-8
 NTE intermediate was isolated

RX(34) RCT BF 901781-68-8
 RGT Q 7719-09-7 SOCl2
 PRO AH 901781-75-7
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

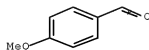
RX(84) OF 139 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
 RX(84) A + B + I + J ==> P



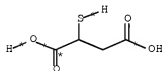
A



B



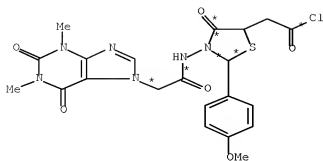
I



J

4
 STEPS
 →

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P
YIELD 43%

RX(1) RCT A 58-55-9
STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

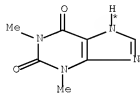
PRO K 901781-44-0
NIE intermediate was isolated

RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

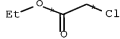
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RX(85) OF 139 COMPOSED OF RX(1), RX(2), RX(21), RX(28)

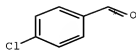
RX(85) A + B + AS + J ==> V



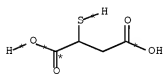
A



B

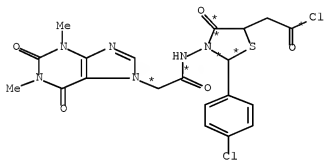


AS



J

4
STEPS
→



V

YIELD 52%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

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RX(2) RCT C 7029-96-1
 RGT G 73603-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

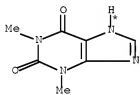
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AT 901781-62-2
 NTE intermediate was isolated

RX(28) RCT AT 901781-62-2
 RGT Q 7719-09-7 SOCl2
 PRO V 901781-69-3
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(86) OF 139 COMPOSED OF RX(1), RX(2), RX(22), RX(29)

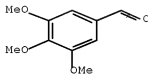
RX(86) A + B + AU + J ==> X



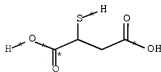
A



B



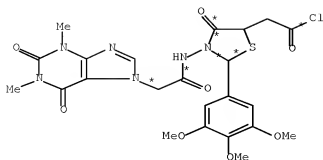
AU



J

4
 STEPS
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X
YIELD 47%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

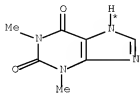
PRO AV 901781-63-3
NTE intermediate was isolated

RX(29) RCT AV 901781-63-3
RGT Q 7719-09-7 SOCl2
PRO X 901781-70-2
SOL 108-88-3 PhMe
CON 30 minutes, reflux

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RX(87) OF 139 COMPOSED OF RX(1), RX(2), RX(23), RX(30)

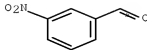
RX(87) A + B + AW + J ==> Z



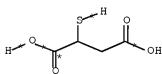
A



B

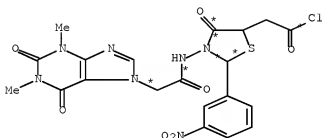


AW



J

4
STEPS
→



Z

YIELD 45%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1

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RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

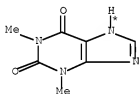
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AX 901781-64-4
 NTE intermediate was isolated

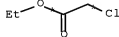
RX(30) RCT AX 901781-64-4
 RGT Q 7719-09-7 SOCl2
 PRO Z 901781-71-3
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(88) OF 139 COMPOSED OF RX(1), RX(2), RX(24), RX(31)

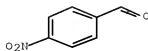
RX(88) A + B + AY + J ==> AB



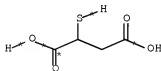
A



B



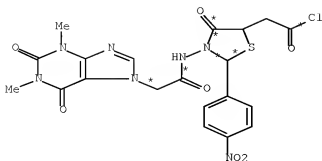
AY



J

4
 STEPS
 →

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AB
YIELD 55%

RX(1) RCT A 58-55-9
STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

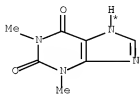
PRO AZ 901781-65-5
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOCl2
PRO AB 901781-72-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

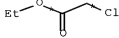
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RX(89) OF 139 COMPOSED OF RX(1), RX(2), RX(25), RX(32)

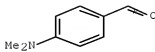
RX(89) A + B + BA + J ==> AD



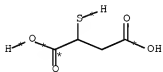
A



B

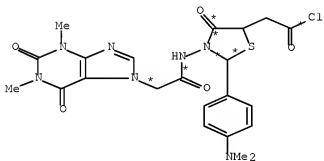


BA



J

4
STEPS
→



AD
YIELD 60%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

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PRO C 7029-96-1

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RX(2)      RCT  C 7029-96-1
           RGT  G 7803-57-8 N2H4-H2O
           PRO  F 41838-25-9
           SOL  123-91-1 Dioxane
           CON  6 hours, reflux

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RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE (1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE (2)

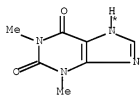
RCT J 70-49-5
CAT 7646-85-7 ZnCl₂
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 901781-66-6

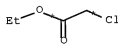
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOC12
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(90) OF 139 COMPOSED OF RX(1), RX(2), RX(26), RX(33)

$$RX(90) \quad A + B + BC + J \implies AF$$


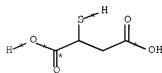
A



B



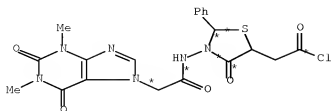
BC



J

4
STEPS
→

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AF
YIELD 48%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2)

RCT C 7029-96-1

RGT G 7803-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

PRO BD 901781-67-7

NTE intermediate was isolated

RX(33)

RCT BD 901781-67-7

RGT Q 7719-09-7 SOCl2

PRO AF 901781-73-6

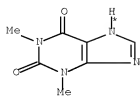
SOL 108-88-3 PhMe

CON 30 minutes, reflux

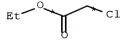
RX(91) OF 139 COMPOSED OF RX(1), RX(2), RX(27), RX(34)

RX(91) A + B + BE + J ==> AH

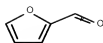
10/595943



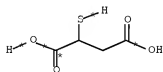
A



B

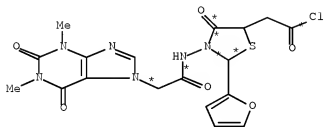


BE



J

4
STEPS
→



AH
YIELD 57%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7646-69-7 N2H4-H2O
PRO F 41838-25-9

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SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

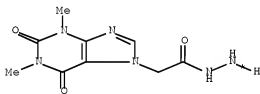
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BF 901781-68-8
NTE intermediate was isolated

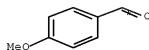
RX(34) RCT BF 901781-68-8
RGT Q 7719-09-7 SOCl2
PRO AH 961781-75-7
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(92) OF 139 COMPOSED OF RX(3), RX(4), RX(5)

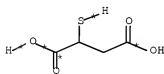
RX(92) F + I + J + S ==> T



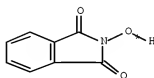
F



I



J



S

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(3) RCT F 41838-25-9, I 123-11-5

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STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 76-46-8b-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

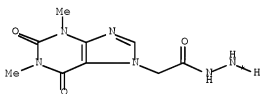
PRO K 901781-44-0
NTE intermediate was isolated

RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

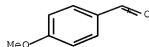
RX(5) RCT P 901781-45-1, S 524-38-9
RGT U 121-44-8 Et3N
PRO T 901781-46-2
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(93) OF 139 COMPOSED OF RX(3), RX(4), RX(13)

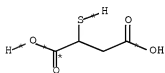
RX(93) F + I + J + AJ ==> AK



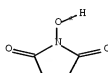
F



I



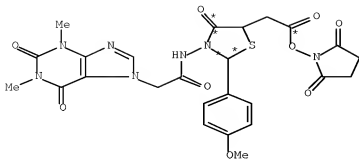
J



AJ

3
STEPS
→

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AK
YIELD 70%

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

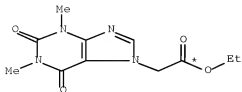
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO K 901781-44-0
NTE intermediate was isolated

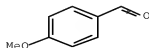
RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(13) RCT P 901781-45-1, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AK 901781-54-2
SOL 68-12-2 DMF
CON 6 hours, room temperature

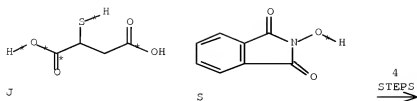
RX(94) OF 139 COMPOSED OF RX(2), RX(3), RX(4), RX(5)
RX(94) C + I + J + S ==> T



C



I



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO K 901781-44-0
 NTE intermediate was isolated

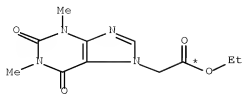
RX(4) RCT K 901781-44-0
 RGT Q 7719-09-7 SOCl2
 PRO P 901781-45-1
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(5) RCT P 901781-45-1, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO T 901781-46-2
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

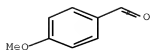
RX(95) OF 139 COMPOSED OF RX(2), RX(3), RX(4), RX(13)

RX(95) C + I + J + AJ ==> AK

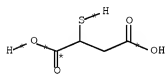
10/595943



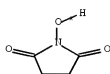
C



I

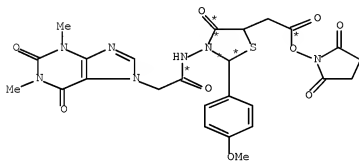


J



AJ

4
STEPS
→



AK
YIELD 70%

RX(2) RCT C 7029-96-1
RGT G 7883-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

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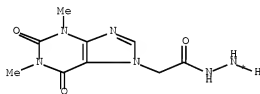
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO K 901781-44-0
NTE intermediate was isolated

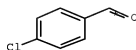
RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(13) RCT P 901781-45-1, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AK 901781-54-2
SOL 68-12-2 DMF
CON 6 hours, room temperature

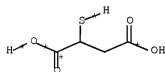
RX(96) OF 139 COMPOSED OF RX(21), RX(28), RX(6)
RX(96) F + AS + J + S ==> W



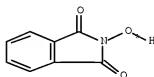
F



AS



J



S

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

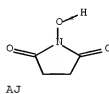
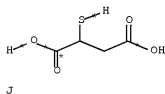
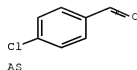
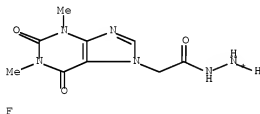
RCT J 70-49-5
 CAT 7546-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AT 901781-62-2
 NTE intermediate was isolated

RX(28) RCT AT 901781-62-2
 RGT Q 7719-09-7 SOCl2
 PRO V 901781-69-9
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

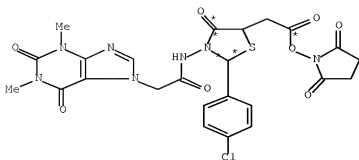
RX(6) RCT V 901781-69-9, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO W 901781-47-3
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(97) OF 139 COMPOSED OF RX(21), RX(28), RX(14)
 RX(97) F + AS + J + AJ ==> AL



3
STEPS
→

10/595943



AL
YIELD 62%

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

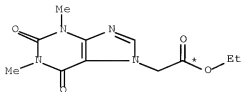
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AT 901781-62-2
NTE intermediate was isolated

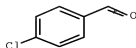
RX(28) RCT AT 901781-62-2
RGT Q 7719-09-7 SOCl2
PRO V 901781-69-9
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(14) RCT V 901781-69-9, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AL 901781-55-3
SOL 68-12-2 DMF
CON 6 hours, room temperature

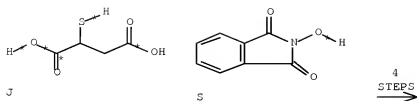
RX(98) OF 139 COMPOSED OF RX(2), RX(21), RX(28), RX(6)
RX(98) C + AS + J + S ==> W



C



AS



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

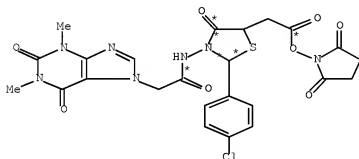
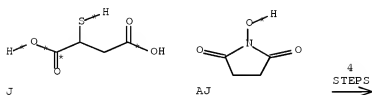
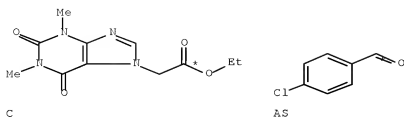
PRO AT 901781-62-2
 NTE intermediate was isolated

RX(28) RCT AT 901781-62-2
 RGT Q 7719-09-7 SOCl2
 PRO V 901781-69-9
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(6) RCT V 901781-69-9, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO W 901781-47-3
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(99) OF 139 COMPOSED OF RX(2), RX(21), RX(28), RX(14)
 RX(99) C + AS + J + AJ ==> AL

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AL
YIELD 62%

RX(2) RCT C 7029-96-1
RGT G 7883-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

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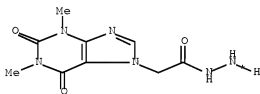
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AT 901781-62-2
NTE intermediate was isolated

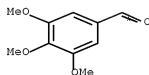
RX(28) RCT AT 901781-62-2
RGT Q 7719-09-7 SOCl2
PRO V 901781-69-9
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(14) RCT V 901781-69-9, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AL 901781-55-3
SOL 68-12-2 DMF
CON 6 hours, room temperature

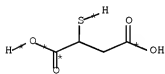
RX(100) OF 139 COMPOSED OF RX(22), RX(29), RX(7)
RX(100) F + AU + J + S ==> Y



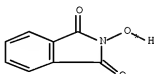
F



AU



J



S

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(22) RCT F 41838-25-5, AU 86-81-7

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

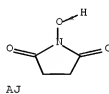
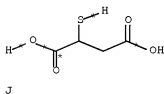
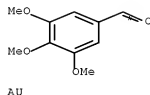
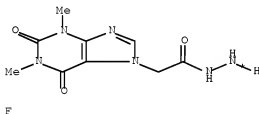
RCT J 70-49-5
 CAT 7546-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AV 901781-63-3
 NTE intermediate was isolated

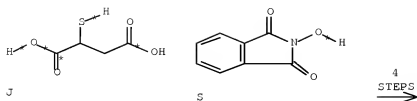
RX(29) RCT AV 901781-63-3
 RGT Q 7719-09-7 SOCl2
 PRO X 901781-70-2
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(7) RCT X 901781-70-2, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO Y 901781-48-4
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(101) OF 139 COMPOSED OF RX(22), RX(29), RX(15)
 RX(101) F + AU + J + AJ ==> AM



3
 STEPS
 →



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AV 901781-63-3
 NTE intermediate was isolated

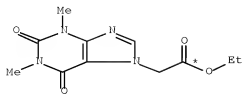
RX(29) RCT AV 901781-63-3
 RGT Q 7719-09-7 SOCl2
 PRO X 901781-70-2
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(7) RCT X 901781-70-2, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO Y 901781-18-4
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

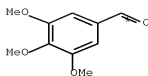
RX(103) OF 139 COMPOSED OF RX(2), RX(22), RX(29), RX(15)

RX(103) C + AU + J + AJ ==> AM

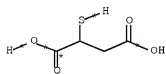
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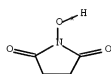
C



AU

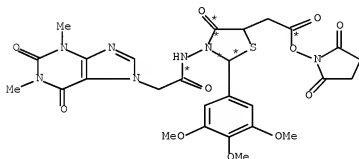


J



AJ

4
STEPS
→



AM
YIELD 64%

RX(2) RCT C 7029-96-1
RGT G 7883-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

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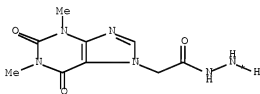
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AV 901781-63-3
NTE intermediate was isolated

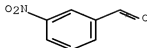
RX(29) RCT AV 901781-63-3
RGT Q 7719-09-7 SOCl2
PRO X 901781-70-2
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(15) RCT X 901781-70-2, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AM 901781-56-4
SOL 68-12-2 DMF
CON 6 hours, room temperature

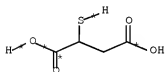
RX(104) OF 139 COMPOSED OF RX(23), RX(30), RX(8)
RX(104) F + AW + J + S ==> AA



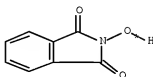
F



AW



J



S

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(23) RCT F 41838-25-2, AW 99-61-6

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

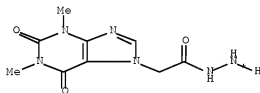
RCT J 70-49-5
 CAT 7546-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AX 901781-64-4
 NTE intermediate was isolated

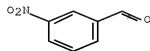
RX(30) RCT AX 901781-64-4
 RGT Q 7719-09-7 SOCl2
 PRO Z 901781-71-3
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(8) RCT Z 901781-71-3, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO AA 901781-49-5
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

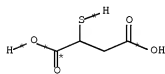
RX(105) OF 139 COMPOSED OF RX(23), RX(30), RX(16)
 RX(105) F + AW + J + AJ ==> AN



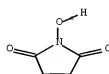
F



AW



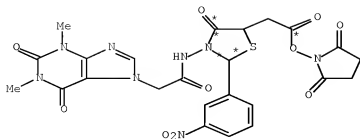
J



AJ

3
 STEPS
 →

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AN
YIELD 73%

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

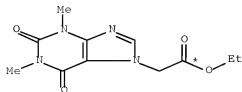
RCT J 70-49-5
CAT 7546-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AX 901781-64-4
NTE intermediate was isolated

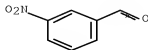
RX(30) RCT AX 901781-64-4
RGT Q 7719-09-7 SOCl2
PRO Z 901781-71-3
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(16) RCT Z 901781-71-3, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AN 901781-57-5
SOL 68-12-2 DMF
CON 6 hours, room temperature

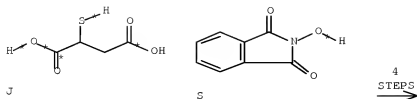
RX(106) OF 139 COMPOSED OF RX(2), RX(23), RX(30), RX(8)
RX(106) C + AW + J + S ==> AA



C



AW



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
 RGT G 7803-57-6 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

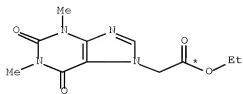
PRO AX 901781-64-4
 NTE intermediate was isolated

RX(30) RCT AX 901781-64-4
 RGT Q 7719-09-7 SOCl2
 PRO Z 901781-71-3
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

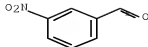
RX(8) RCT Z 901781-71-3, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO AA 901781-49-5
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(107) OF 139 COMPOSED OF RX(2), RX(23), RX(30), RX(16)
 RX(107) C + AW + J + AJ ==> AN

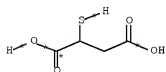
10/595943



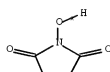
C



AW

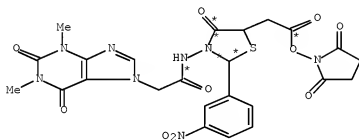


J



AJ

4
STEPS
→



AN
YIELD 73%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2

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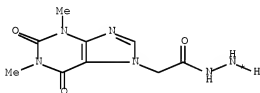
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AX 901781-64-4
NTE intermediate was isolated

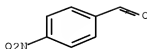
RX(30) RCT AX 901781-64-4
RGT Q 7719-09-7 SOCl2
PRO Z 901781-71-3
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(16) RCT Z 901781-71-3, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AN 901781-57-5
SOL 68-12-2 DMF
CON 6 hours, room temperature

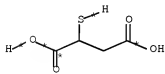
RX(108) OF 139 COMPOSED OF RX(24), RX(31), RX(9)
RX(108) F + AY + J + S ==> AC



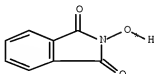
F



AY



J



S

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

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STAGE (2)

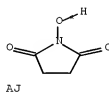
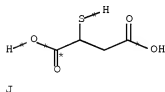
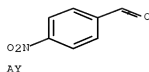
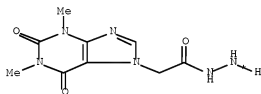
RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO AZ 901781-65-5
 NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5
 RGT Q 7719-09-7 SOCl2
 PRO AB 901781-72-4
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

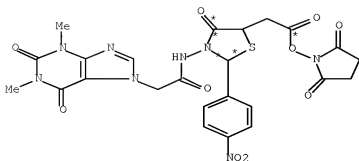
RX(9) RCT AB 901781-72-4, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO AC 901781-50-8
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(109) OF 139 COMPOSED OF RX(24), RX(31), RX(17)
 RX(109) F + AY + J + AJ ==> AO



3
 STEPS
 →

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AO
YIELD 69%

RX(24) RCT F 41638-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

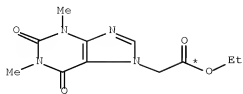
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AZ 901781-65-5
NTE intermediate was isolated

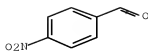
RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOCl2
PRO AB 901781-72-4
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(17) RCT AB 901781-72-4, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AO 901781-58-6
SOL 68-12-2 DMF
CON 6 hours, room temperature

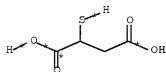
RX(110) OF 139 COMPOSED OF RX(2), RX(24), RX(31), RX(9)
RX(110) C + AY + J + S ==> AC



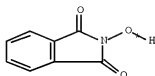
C



AY



J



S

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
RGT G 7663-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AZ 901781-65-5
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOCl2
PRO AB 901781-72-4
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(9) RCT AB 901781-72-4, S 524-38-9
RGT U 121-44-8 Et3N

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RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

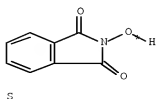
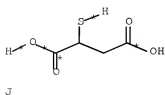
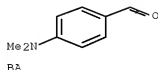
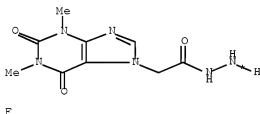
RCT J 73-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AZ 901781-65-5
NTE intermediate was isolated

RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOCl2
PRO AB 901781-72-4
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(17) RCT AB 901781-72-4, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AO 901781-58-6
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(112) OF 139 COMPOSED OF RX(25), RX(32), RX(10)
RX(112) F + BA + J + S ==> AE



3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

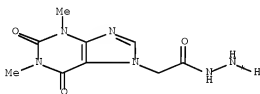
PRO BB 901781-66-6
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOCl2
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

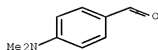
RX(10) RCT AD 901781-73-5, S 524-38-9
RGT U 121-44-8 Et3N
PRO AE 901781-51-9
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(113) OF 139 COMPOSED OF RX(25), RX(32), RX(18)

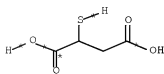
RX(113) F + BA + J + AJ ==> AF



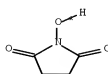
F



BA

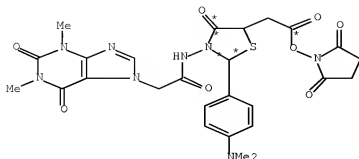


J



AJ

3
STEPS
→



AP
YIELD 62%

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-85-7 ZnCl2

SOL 109-99-9 THF

CON 10 hours, reflux

PRO BB 901781-66-6

NTE intermediate was isolated

RX(32) RCT BB 901781-66-6

RGT Q 7719-09-7 SOCl2

PRO AD 901781-73-5

SOL 108-88-3 PhMe

CON 30 minutes, reflux

RX(18) RCT AD 901781-73-5, AJ 6066-82-6

RGT U 121-44-8 Et3N

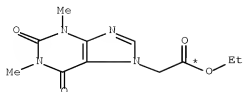
PRO AP 901781-59-7

SOL 68-12-2 DMF

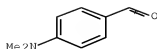
CON 6 hours, room temperature

RX(114) OF 139 COMPOSED OF RX(2), RX(25), RX(32), RX(10)

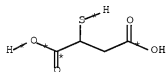
RX(114) C + BA + J + S ==> AE



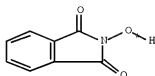
C



BA



J



S

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
RGT G 7663-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 901781-66-6
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOCl2
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(10) RCT AD 901781-73-5, S 524-38-9
RGT U 121-44-8 Et3N

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RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

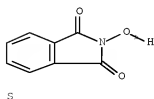
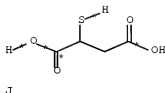
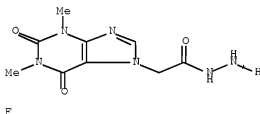
RCT J 73-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 901781-66-6
NTE intermediate was isolated

RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOCl2
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

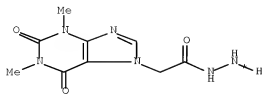
RX(18) RCT AD 901781-73-5, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AP 901781-59-7
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(116) OF 139 COMPOSED OF RX(26), RX(33), RX(11)
RX(116) F + BC + J + S ==> AG



3
STEPS
→

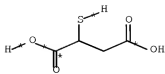
10/595943



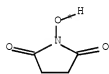
F



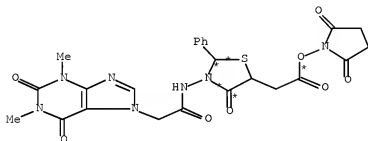
BC



J



AJ



AQ
YIELD 68%

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 78-49-5
CAT 7546-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BD 901781-67-7

NTE intermediate was isolated

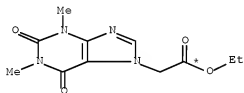
10/595943

RX(33) RCT BD 901781-67-7
 RGT Q 7719-09-7 SOCl2
 PRO AF 901781-74-6
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(19) RCT AF 901781-74-6, AJ 6066-82-6
 RGT U 121-44-8 Et3N
 PRO AQ 901781-60-0
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(118) OF 139 COMPOSED OF RX(2), RX(26), RX(33), RX(11)

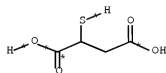
RX(118) C + BC + J + S ==> AG



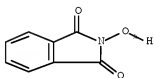
C



BC

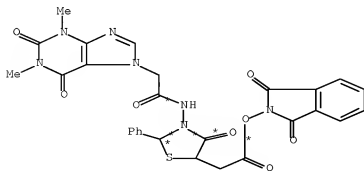


J



S

4
STEPS
→



AG
 YIELD 60%

RX(2) RCT C 7029-96-1
 RGT G 7893-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

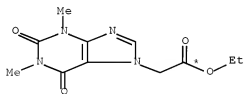
STAGE(2)
 RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO BD 901781-67-7
 NTE intermediate was isolated

RX(33) RCT BD 901781-67-7
 RGT Q 7719-09-7 SOCl2
 PRO AF 901781-74-6
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(11) RCT AF 901781-74-6, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO AG 901781-52-0
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

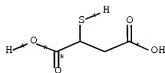
RX(119) OF 139 COMPOSED OF RX(2), RX(26), RX(33), RX(19)
 RX(119) C + BC + J + AJ ==> RQ



C

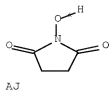


BC

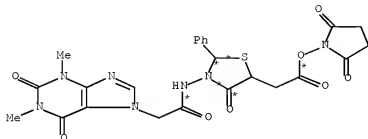


J

10/595943



4
STEPS
→



AQ
YIELD 68%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BD 901781-67-7
NTE intermediate was isolated

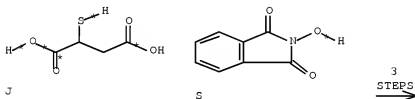
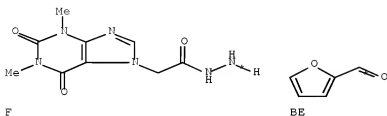
RX(33) RCT BD 901781-67-7
RGT Q 7719-09-7 SOCl2
PRO AF 901781-74-6
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(19) RCT AF 901781-74-6, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AQ 901781-60-0

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SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(120) OF 139 COMPOSED OF RX(27), RX(34), RX(12)
RX(120) F + BE + J + S ==> AI



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

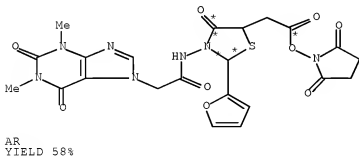
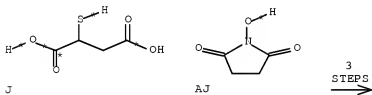
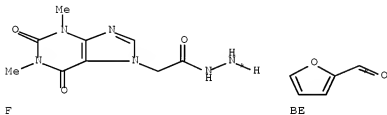
PRO BF 901781-68-8
NIE intermediate was isolated

RX(34) RCT BF 901781-68-8
RGT Q 7719-09-7 SOCl2
PRO AH 901781-75-7
SOL 108-88-3 PhMe
CON 30 minutes, reflux

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RX(12) RCT AH 901781-75-7, S 524-38-9
RGT U 121-44-8 Et3N
PRO AI 901781-53-1
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(121) OF 139 COMPOSED OF RX(27), RX(34), RX(20)
RX(121) F + BE + J + AJ ==> AR



RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE (1)

CAT	64-19-7	AcOH
SOL	64-17-5	EtOH
CON	5 hours,	reflux

STAGE(2)

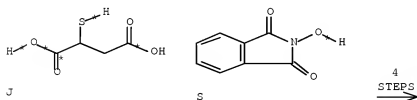
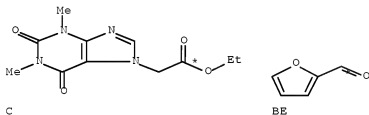
RCT J 70-49-5
 CAT 7546-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO BF 901781-68-8
 NTE intermediate was isolated

RX(34) RCT BF 901781-68-8
 RGT Q 7719-09-7 SOCl2
 PRO AH 901781-75-7
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(20) RCT AH 901781-75-7, AJ 6066-82-6
 RGT U 121-44-8 Et3N
 PRO AR 901781-61-1
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(122) OF 139 COMPOSED OF RX(2), RX(27), RX(34), RX(12)
 RX(122) C + BE + J + S ==> AI



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9

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SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

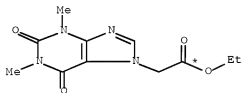
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BF 901781-68-8
NTE intermediate was isolated

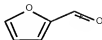
RX(34) RCT BF 901781-68-8
RGT Q 7719-09-7 SOCl2
PRO AH 901781-75-7
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(12) RCT AH 901781-75-7, S 524-38-9
RGT U 121-44-8 Et3N
PRO AI 901781-53-1
SOL 68-12-2 DMF
CON 6 hours, room temperature

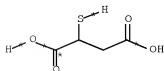
RX(123) OF 139 COMPOSED OF RX(2), RX(27), RX(34), RX(20)
RX(123) C + BE + J + AJ ==> AR



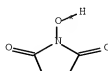
C



BE

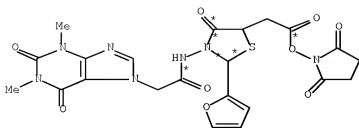


J



AJ

4
STEPS
→



AR
YIELD 58%

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

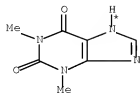
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BF 901781-68-8
NTE intermediate was isolated

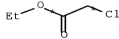
RX(34) RCT BF 901781-68-8
RGT Q 7719-09-7 SOCl2
PRO AH 901781-75-7
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(20) RCT AH 901781-75-7, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AR 901781-61-1
SOL 68-12-2 DMF
CON 6 hours, room temperature

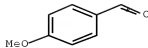
RX(124) OF 139 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)
RX(124) A + B + I + J + S ==> T



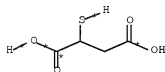
A



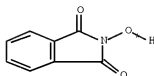
B



I



J



S



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2)

RCT C 7029-96-1

RGT G 7803-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(3)

RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5

CAT 7646-69-7 ZnCl2

SOL 109-99-9 THF

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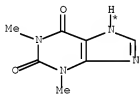
CON 10 hours, reflux

PRO K 901781-44-0
NTE intermediate was isolated

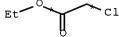
RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOC12
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(5) RCT P 901781-45-1, S 524-38-9
RGT U 121-44-8 Et3N
PRO T 901781-46-2
SOL 68-12-2 DMF
CON 6 hours, room temperature

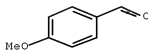
RX(125) OF 139 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13)
RX(125) A + B + I + J + AJ ==> AK



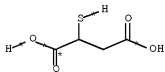
A



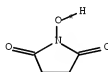
B



I

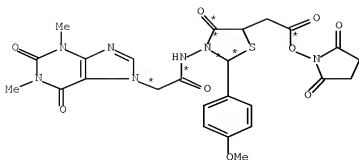


J



AJ

5
STEPS
→



AK
YIELD 70%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(3) RCT F 41838-25-9, I 123-11-5

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO K 901781-44-0
NTE intermediate was isolated

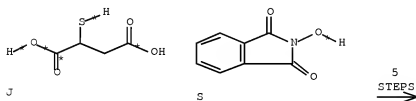
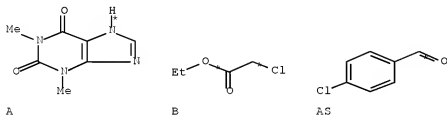
RX(4) RCT K 901781-44-0
RGT Q 7719-09-7 SOCl2
PRO P 901781-45-1
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(13) RCT P 901781-45-1, AJ 6066-82-6

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RGT U 121-44-8 Et3N
 PRO AK 961781-54-2
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(126) OF 139 COMPOSED OF RX(1), RX(2), RX(21), RX(28), RX(6)
 RX(126) A + B + AS + J + S ==> W



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
 CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

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STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

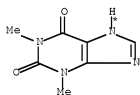
RCT J 76-49-5
CAT 76-46-8b-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AT 901781-62-2
NTE intermediate was isolated

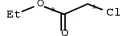
RX(28) RCT AT 901781-62-2
RGT Q 7719-09-7 SOCl2
PRO V 901781-69-9
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(6) RCT V 901781-69-9, S 524-38-9
RGT U 121-44-8 Et3N
PRO W 901781-47-3
SOL 68-12-2 DMF
CON 6 hours, room temperature

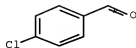
RX(127) OF 139 COMPOSED OF RX(1), RX(2), RX(21), RX(28), RX(14)
RX(127) A + B + AS + J + AJ ==> AL



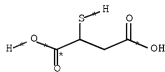
A



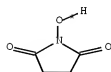
B



AS

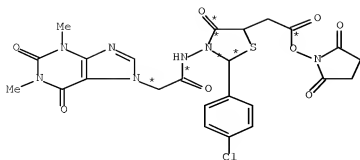


J



AJ

5
STEPS
→



AL
YIELD 62%

RX(1) RCT A 58-55-9

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(21) RCT F 41838-25-9, AS 104-88-1

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AT 901781-62-2
NIE intermediate was isolated

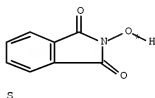
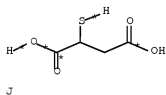
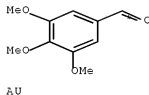
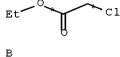
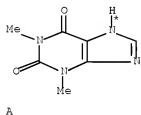
RX(28) RCT AT 901781-62-2
RGT Q 7719-09-7 SOCl2
PRO V 901781-69-9
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(14) RCT V 901781-69-9, AJ 6066-82-6

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RGT U 121-44-8 Et3N
 PRO AL 961781-55-3
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(128) OF 139 COMPOSED OF RX(1), RX(2), RX(22), RX(29), RX(7)
 RX(128) A + B + AU + J + S ==> Y



5
 STEPS
 →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
 CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

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STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

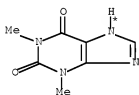
RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AV 901781-63-3
NTE intermediate was isolated

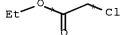
RX(29) RCT AV 901781-63-3
RGT Q 7719-09-7 SOCl2
PRO X 901781-70-2
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(7) RCT X 901781-70-2, S 524-38-9
RGT U 121-44-8 Et3N
PRO Y 901781-48-4
SOL 68-12-2 DMF
CON 6 hours, room temperature

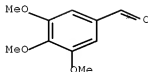
RX(129) OF 139 COMPOSED OF RX(1), RX(2), RX(22), RX(29), RX(15)
RX(129) A + B + AU + J + AJ ==> AM



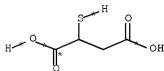
A



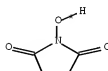
B



AU

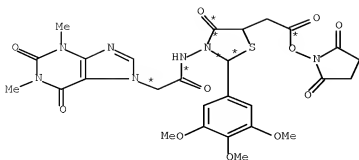


J



AJ

5
STEPS
→



AM
YIELD 64%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(22) RCT F 41838-25-9, AU 86-81-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AV 901781-63-3
NTE intermediate was isolated

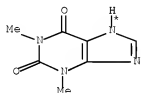
RX(29) RCT AV 901781-63-3
RGT Q 7719-09-7 SOCl2
PRO X 901781-70-2
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(15) RCT X 901781-70-2, AJ 6066-82-6

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RGT U 121-44-8 Et3N
 PRO AM 961781-56-4
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

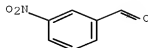
RX(130) OF 139 COMPOSED OF RX(1), RX(2), RX(23), RX(30), RX(8)
 RX(130) A + B + AW + J + S ==> AA



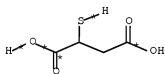
A



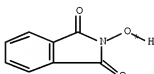
B



AW



J



S

5
 STEPS
 →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
 CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
 RGT G 7803-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(23) RCT F 41838-25-9, AW 99-61-6

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STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 76-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

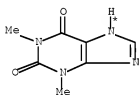
PRO AX 901781-64-4
NTE intermediate was isolated

RX(30) RCT AX 901781-64-4
RGT Q 7719-09-7 SOCl2
PRO Z 901781-71-3
SOL 108-88-3 PhMe
CON 30 minutes, reflux

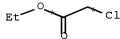
RX(8) RCT Z 901781-71-3, S 524-38-9
RGT U 121-44-8 Et3N
PRO AA 901781-49-5
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(131) OF 139 COMPOSED OF RX(1), RX(2), RX(23), RX(30), RX(16)

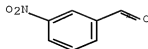
RX(131) A + B + AW + J + AJ ==> AN



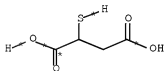
A



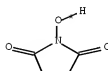
B



AW



J



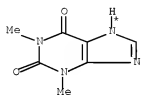
AJ

5
STEPS
→

10/595943

PRO AN 901781-57-5
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

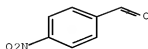
RX(132) OF 139 COMPOSED OF RX(1), RX(2), RX(24), RX(31), RX(9)
 RX(132) A + B + AY + J + S ==> PC



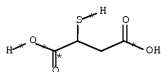
A



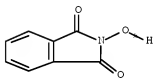
B



AY



J



S

5
 STEPS
 →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)
 RGT D 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 2 hours, room temperature

STAGE(2)
 RCT B 105-39-5
 CON 6 hours, reflux

10/595943

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7883-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

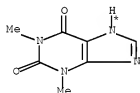
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AZ 901781-65-5
NTE intermediate was isolated

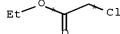
RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOCl2
PRO AB 901781-72-4
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(9) RCT AB 901781-72-4, S 524-38-9
RGT U 121-44-8 Et3N
PRO AC 901781-50-8
SOL 68-12-2 DMF
CON 6 hours, room temperature

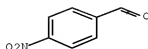
RX(133) OF 139 COMPOSED OF RX(1), RX(2), RX(24), RX(31), RX(17)
RX(133) A + B + AY + J + AJ ==> AO



A

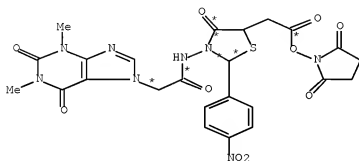
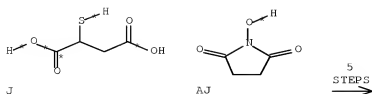


B



AY

10/595943



AO
YIELD 69%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2)

RCT C 7029-96-1

RGT G 7863-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(24) RCT F 41838-25-9, AY 555-16-8

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 78-49-5

CAT 7646-85-7 ZnCl2

10/595943

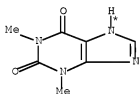
SOL 109-99-9 THF
CON 10 hours, reflux

PRO AZ 901781-65-5
NTE intermediate was isolated

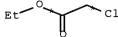
RX(31) RCT AZ 901781-65-5
RGT Q 7719-09-7 SOC12
PRO AB 901781-72-4
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(17) RCT AB 901781-72-4, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AO 901781-58-6
SOL 68-12-2 DMF
CON 6 hours, room temperature

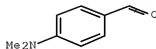
RX(134) OF 139 COMPOSED OF RX(1), RX(2), RX(25), RX(32), RX(10)
RX(134) A + B + BA + J + S ==> AE



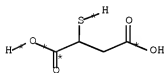
A



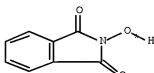
B



BA



J



S

5
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)

10/595943

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7003-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

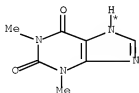
PRO BB 901781-66-6

NTE intermediate was isolated

RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOCl2
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(10) RCT AD 901781-73-5, S 524-38-9
RGT U 121-44-8 Et3N
PRO AE 901781-51-9
SOL 68-12-2 DMF
CON 6 hours, room temperature

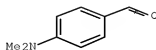
RX(135) OF 139 COMPOSED OF RX(1), RX(2), RX(25), RX(32), RX(18)
RX(135) A + B + BA + J + AJ ==> AP



A

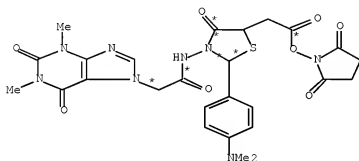
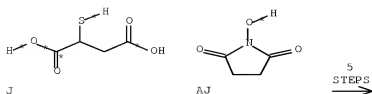


B



BA

10/595943



AP
YIELD 62%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5

CON 6 hours, reflux

PRO C 7029-96-1

RX(2)

RCT C 7029-96-1

RGT G 7863-57-8 N2H4-H2O

PRO F 41838-25-9

SOL 123-91-1 Dioxane

CON 6 hours, reflux

RX(25) RCT F 41838-25-9, BA 100-10-7

STAGE(1)

CAT 64-19-7 AcOH

SOL 64-17-5 EtOH

CON 5 hours, reflux

STAGE(2)

RCT J 78-49-5

CAT 7646-85-7 ZnCl2

10/595943

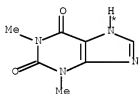
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BB 901781-66-6
NTE intermediate was isolated

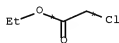
RX(32) RCT BB 901781-66-6
RGT Q 7719-09-7 SOC12
PRO AD 901781-73-5
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(18) RCT AD 901781-73-5, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AP 901781-59-7
SOL 68-12-2 DMF
CON 6 hours, room temperature

RX(136) OF 139 COMPOSED OF RX(1), RX(2), RX(26), RX(33), RX(11)
RX(136) A + B + BC + J + S ==> AG



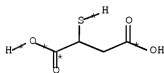
A



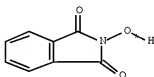
B



BC



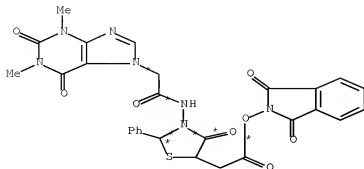
J



S

5
STEPS
→

10/595943



AG
YIELD 60%

RX(1) RCT A 58-55-9
STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)
RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)
RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

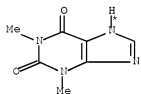
PRO BD 901781-67-7
NTE intermediate was isolated

RX(33) RCT BD 901781-67-7
RGT Q 7719-09-7 SOCl2
PRO AF 901781-74-6
SOL 108-88-3 PhMe
CON 30 minutes, reflux

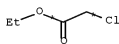
10/595943

RX(11) RCT AF 901781-74-6, S 524-38-9
 RGT U 121-44-8 Et3N
 PRO AG 901781-52-0
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

RX(137) OF 139 COMPOSED OF RX(1), RX(2), RX(26), RX(33), RX(19)
 RX(137) A + B + BC + J + AJ ==> AQ



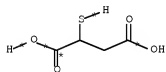
A



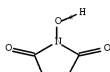
B



BC

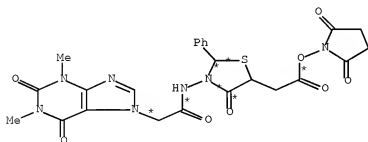


J



AJ

5
STEPS
→



AQ
 YIELD 68%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(26) RCT F 41838-25-9, BC 100-52-7

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

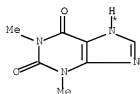
RCT J 79-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BD 901781-67-7
NTE intermediate was isolated

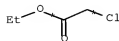
RX(33) RCT BD 901781-67-7
RGT Q 7719-09-7 SOCl2
PRO AF 901781-74-6
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(19) RCT AF 901781-74-6, AJ 6066-82-6
RGT U 121-44-8 Et3N
PRO AQ 901781-60-0
SOL 68-12-2 DMF
CON 6 hours, room temperature

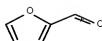
RX(138) OF 139 COMPOSED OF RX(1), RX(2), RX(27), RX(34), RX(12)
RX(138) A + B + BE + J + S ==> AI



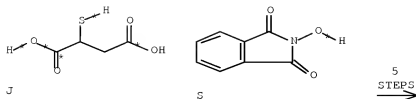
A



B



BE



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
RGT G 7803-57-8 N2H4-H2O
PRO F 41838-25-9
SOL 123-91-1 Dioxane
CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 5 hours, reflux

STAGE(2)

RCT J 70-49-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 10 hours, reflux

PRO BF 901781-68-8
NTE intermediate was isolated

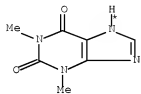
RX(34) RCT BF 901781-68-8
RGT Q 7719-09-7 SOCl2
PRO AH 901781-75-7
SOL 108-88-3 PhMe
CON 30 minutes, reflux

RX(12) RCT AH 901781-75-7, S 524-38-9
RGT U 121-44-8 Et3N
PRO AI 901781-53-1

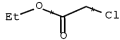
10/595943

SOL 68-12-2 DMF
CON 6 hours, room temperature

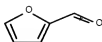
RX(139) OF 139 COMPOSED OF RX(1), RX(2), RX(27), RX(34), RX(20)
RX(139) A + B + BE + J + AJ ==> AP



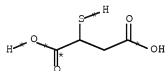
A



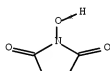
B



BE

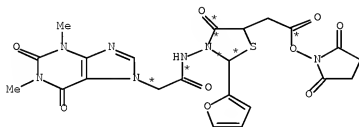


J



AJ

5
STEPS
→



AP
YIELD 58%

RX(1) RCT A 58-55-9

STAGE(1)

RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON 2 hours, room temperature

STAGE(2)

RCT B 105-39-5
CON 6 hours, reflux

PRO C 7029-96-1

RX(2) RCT C 7029-96-1
 RGT G 7893-57-8 N2H4-H2O
 PRO F 41838-25-9
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(27) RCT F 41838-25-9, BE 98-01-1

STAGE(1)
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 5 hours, reflux

STAGE(2)
 RCT J 70-49-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 10 hours, reflux

PRO BF 901781-68-8
 NIE intermediate was isolated

RX(34) RCT BF 901781-68-8
 RGT Q 7719-09-7 SOCl2
 PRO AH 901781-75-7
 SOL 108-88-3 PhMe
 CON 30 minutes, reflux

RX(20) RCT AH 901781-75-7, AJ 6066-82-6
 RGT U 121-44-8 Et3N
 PRO AR 901781-61-1
 SOL 68-12-2 DMF
 CON 6 hours, room temperature

L91 ANSWER 4 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:62814 CASREACT [Full-text](#)

TITLE: Synthesis and antimicrobial activity of phthalimido
 (2-aryl-3-isonicotinamido-4-oxo-1,3-thiazolidin-5-
 yl)ethanoates

AUTHOR(S): Sharma, Ranjana; Ahmed, M.; Sharma, Kanika; Talesara,
 G. L.

CORPORATE SOURCE: Department of Botany and Department of Chemistry, M.
 L. Sukhadia University, Udaipur, 313 001, India

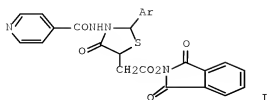
SOURCE: Indian Journal of Pharmaceutical Sciences (2005),
 67(4), 462-466
 CODEN: IJPSIDW; ISSN: 0250-474X

PUBLISHER: Indian Pharmaceutical Association

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

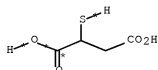
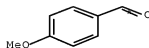
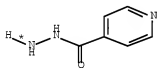


AB Title compds. I [Ar = (un)substituted Ph, 2-furanyl] were prepared in 4 steps starting from isoniazid and ArCHO and including a heterocyclization reaction of mercaptosuccinic acid. All the synthesized compds. were screened for antibacterial (*Bacillus subtilis*, *Escherichia coli*, *Klebsiella pneumoniae*, *Proteus vulgaris*, *Pseudomonas aeruginosa* and *Salmonella typhi*) and antifungal (*Candida albicans* and *Aspergillus fumigatus*) activities. All the compds. exhibited significant activity against the bacteria and fungi tested.

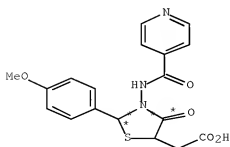
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(33) OF 80 COMPOSED OF RX(1), RX(9)

RX(33) A + B + T ==> U



2
STEPS
→



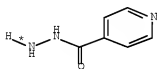
YIELD 78%

10/595943

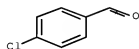
RX(1) RCT A 54-85-3, B 123-11-5
 RGT D 64-19-7 AcOH
 PRO C 893-42-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(9) RCT C 893-42-5, T 70-49-5
 PRO U 103706-40-7
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 8 hours, reflux

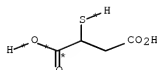
RX(34) OF 80 COMPOSED OF RX(2), RX(10)
 RX(34) A + F + T ==> X



A

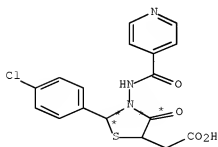


F



T

2
 STEPS
 →



X
 YIELD 71%

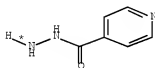
RX(2) RCT A 54-85-3, F 104-88-1
 RGT D 64-19-7 AcOH

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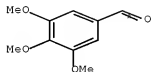
PRO G 6342-46-7
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(10) RCT G 6342-46-7, T 70-49-5
PRO X 193710-50-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

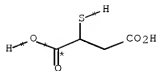
RX(35) OF 80 COMPOSED OF RX(3), RX(11)
RX(35) A + H + T ==> Y



A

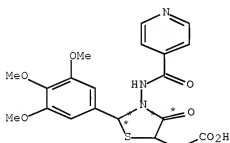


H



T

2
STEPS
→



Y
YIELD 70%

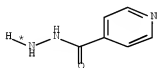
RX(3) RCT A 54-85-3, H 86-81-7
RGT D 64-19-7 AcOH
PRO I 67837-40-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(11) RCT I 67837-40-5, T 70-49-5
PRO Y 859948-58-5

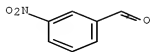
10/595943

CAT 7546-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

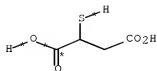
RX(36) OF 80 COMPOSED OF RX(4), RX(12)
RX(36) A + J + T ==> Z



A

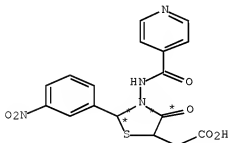


J



T

2
STEPS
→



Z
YIELD 73%

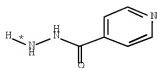
RX(4) RCT A 54-85-3, J 99-61-6
RGT D 64-19-7 AcOH
PRO K 16012-26-3
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(12) RCT K 16012-26-3, T 70-49-5
PRO Z 101706-31-6
CAT 7546-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

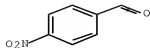
RX(37) OF 80 COMPOSED OF RX(5), RX(13)

10/595943

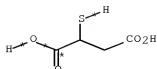
RX(37) A + L + T ==> AA



A

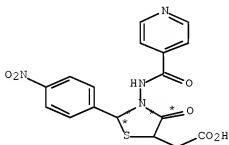


L



T

2
STEPS
→



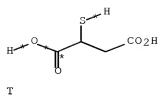
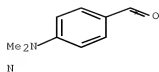
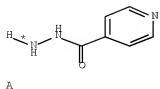
AA
YIELD 76%

RX(5) RCT A 54-25-3, L 555-16-8
 RGT D 64-19-7 AcOH
 PRO M 4813-07-4
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

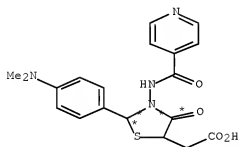
RX(13) RCT M 4813-07-4, T 70-49-5
 PRO AA 103706-32-7
 CAT 7646-25-7 ZnCl2
 SOL 109-99-9 THF
 CON 8 hours, reflux

RX(38) OF 80 COMPOSED OF RX(6), RX(14)
 RX(38) A + N + T ==> AB

10/595943



2
STEPS
→



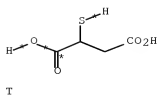
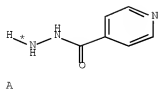
AB
YIELD 74%

RX(6) RCT A 54-85-3, N 100-10-7
RGT D 64-19-7 AcOH
PRO O 13059-77-3
SOL 64-17-5 EtOH
CON 4 hours, reflux

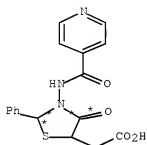
RX(14) RCT O 13059-77-3, T 70-49-5
PRO AB 93607-15-9
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(39) OF 80 COMPOSED OF RX(7), RX(15)
RX(39) A + P + T ==> AC

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2
STEPS
→

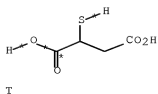
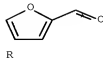
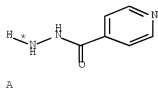


AC
YIELD 69%

RX(7) RCT A 54-35-3, P 100-52-7
RGT D 64-19-7 AcOH
PRO Q 533-02-8
SOL 64-17-5 EtOH
CON 4 hours, reflux

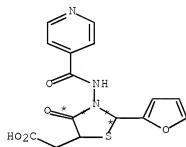
RX(15) RCT Q 533-02-8, T 70-43-5
PRO AC 24327-74-8
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(40) OF 80 COMPOSED OF RX(8), RX(16)
RX(40) A + R + T ==> AD



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2
STEPS
→

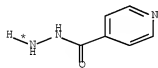


AD
YIELD 65%

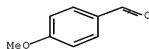
RX(8) RCT A 54-95-3, R 98-01-1
RGT D 64-19-7 AcOH
PRO S 6956-53-2
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(16) RCT S 6956-53-2, T 78-49-5
PRO AD 183706-42-9
CAT 7646-95-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

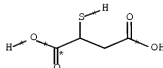
RX(57) OF 80 COMPOSED OF RX(1), RX(9), RX(17)
RX(57) A + B + T ==> AE



A

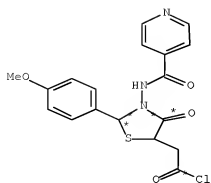


B



T

3
STEPS
→



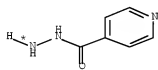
AE
YIELD 62%

RX(1) RCT A 54-85-3, B 123-11-5
RGT D 64-19-7 AcOH
PRO C 893-42-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

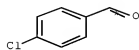
RX(9) RCT C 893-42-5, T 70-49-5
PRO U 103706-40-7
CAT 76-46-8 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(17) RCT U 103706-40-7
RGT AF 7719-09-7 SOCl2
PRO AE 830948-59-6
SOL 71-43-2 Benzene
CON 60 minutes, reflux

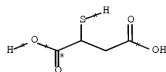
RX(58) OF 80 COMPOSED OF RX(2), RX(10), RX(18)
RX(58) A + F + T ==> AE



A

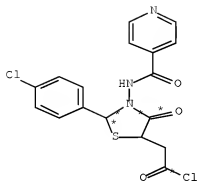


F



T

3
STEPS
→



AH
YIELD 60%

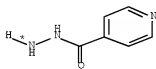
RX(2) RCT A 54-85-3, F 104-88-1
RGT D 64-19-7 AcOH
PRO G 6342-46-7
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(10) RCT G 6342-46-7, T 70-49-5
PRO X 103710-50-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

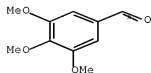
RX(18) RCT X 103710-50-5
RGT AF 7719-09-7 SOCl2
PRO AH 890848-60-9
SOL 71-43-2 Benzene
CON 60 minutes, reflux

RX(59) OF 80 COMPOSED OF RX(3), RX(11), RX(19)

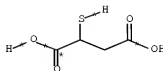
RX(59) A + H + T ==> AJ



A



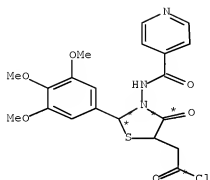
H



T

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3
STEPS
→



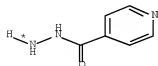
AI
YIELD 66%

RX(3) RCT A 54-85-3, H 86-81-7
RGT D 64-19-7 AcOH
PRO I 67837-40-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

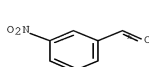
RX(11) RCT I 67837-40-5, T 70-49-5
PRO Y 890848-58-5
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(19) RCT Y 890848-58-5
RGT AF 7719-09-7 SOCl2
PRO AI 890848-61-0
SOL 71-43-2 Benzene
CON 60 minutes, reflux

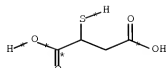
RX(60) OF 80 COMPOSED OF RX(4), RX(12), RX(20)
RX(60) A + J + T ==> AJ



A

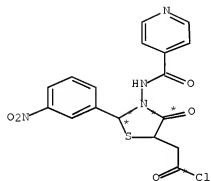


J



T

3
STEPS
→



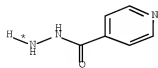
AJ
YIELD 58%

RX(4) RCT A 54-85-3, J 99-61-6
RGT D 64-19-7 AcOH
PRO K 16012-26-3
SOL 64-17-5 EtOH
CON 4 hours, reflux

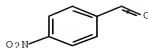
RX(12) RCT K 16012-26-3, T 70-49-5
PRO Z 103706-31-6
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(20) RCT Z 103706-31-6
RGT AF 7719-09-7 SOCl2
PRO AJ 890848-62-1
SOL 71-43-2 Benzene
CON 60 minutes, reflux

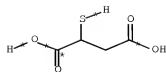
RX(61) OF 80 COMPOSED OF RX(5), RX(13), RX(21)
RX(61) A + L + T ==> AK



A

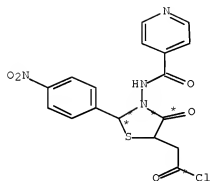


L



T

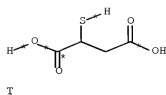
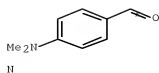
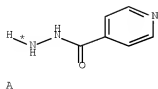
3
STEPS
→



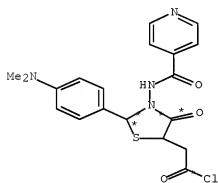
AK
YIELD 55%

RX(5)	RCT	A 54-95-3, L 555-16-8
	RGT	D 64-19-7 AcOH
	PRO	M 4813-07-4
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(13)	RCT	M 4813-07-4, T 70-49-5
	PRO	AA 103706-32-7
	CAT	7646-85-7 ZnCl2
	SOL	109-99-9 THF
	CON	8 hours, reflux
RX(21)	RCT	AA 103706-32-7
	RGT	AF 7719-09-7 SOCl2
	PRO	AK 890848-63-2
	SOL	71-43-2 Benzene
	CON	60 minutes, reflux
RX(62) OF 80 COMPOSED OF RX(6), RX(14), RX(22)		
RX(62)	A	+ N + T ==> AL

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3
STEPS
→



AL
YIELD 67%

RX(6) RCT A 54-85-3, N 100-10-7
RGT D 64-19-7 AcOH
PRO O 13059-77-3
SOL 64-17-5 EtOH
CON 4 hours, reflux

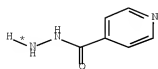
RX(14) RCT O 13059-77-3, T 70-49-5
PRO AB 93607-15-9
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(22) RCT AB 93607-15-9
RGT AF 7719-09-7 SOCl2
PRO AL 898848-64-3
SOL 71-43-2 Benzene
CON 60 minutes, reflux

RX(63) OF 80 COMPOSED OF RX(7), RX(15), RX(23)

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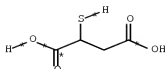
RX(63) A + P + T ==> AM



A

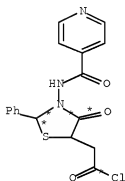


P



T

3
STEPS
→



AM
YIELD 53%

RX(7) RCT A 54-85-3, P 100-52-7
RGT D 64-19-7 AcOH
PRO Q 533-02-8
SOL 64-17-5 EtOH
CON 4 hours, reflux

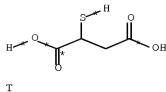
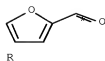
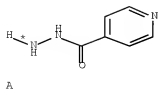
RX(15) RCT Q 533-02-8, T 70-49-5
PRO AC 24327-74-0
CAT 7646-95-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(23) RCT AC 24327-74-0
RGT AF 7719-09-7 SOCl2
PRO AM 890848-65-4
SOL 71-43-2 Benzene
CON 60 minutes, reflux

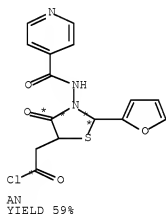
RX(64) OF 80 COMPOSED OF RX(8), RX(16), RX(24)

RX(64) A + R + T ==> AM

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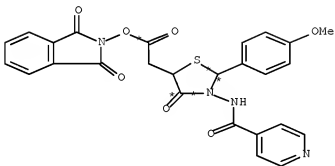
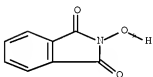
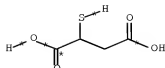
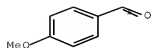
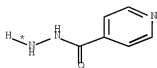
3
STEPS
→



RX(8)	RCT	A 54-85-3, R 98-01-1
	RGT	D 64-19-7 AcOH
	PRO	S 6956-53-2
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(16)	RCT	S 6956-53-2, T 70-49-5
	PRO	AD 103706-42-9
	CAT	7646-85-7 ZnCl2
	SOL	109-99-9 THF
	CON	8 hours, reflux
RX(24)	RCT	AD 103706-42-9
	RGT	AF 7719-09-7 SOCl2
	PRO	AN 6956-53-2
	SOL	71-43-2 Benzene
	CON	60 minutes, reflux

RX(66) OF 80 COMPOSED OF RX(1), RX(9), RX(17), RX(25)

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$$\text{RX(66)} \quad \text{A} + \text{B} + \text{T} + \text{AO} \implies \text{AP}$$


RX(1) RCT A 54-85-3, B 123-11-5
RGT D 64-19-7 AcOH
PRO C 893-42-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(9) RCT C 893-42-5, T 70-49-5
PRO U 103706-40-7
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

RX(17) RCT U 103706-40-7

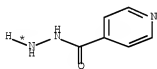
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RGT AF 7719-09-7 SOC12
 PRO AE 890848-59-6
 SOL 71-43-2 Benzene
 CON 60 minutes, reflux

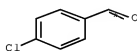
RX(25) RCT AE 890848-59-6, AO 524-38-9
 RGT AQ 121-44-8 Et3N
 PRO AP 890848-67-6
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 3 hours, reflux

RX(68) OF 80 COMPOSED OF RX(2), RX(10), RX(18), RX(26)

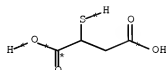
RX(68) A + F + T + AO ==> AS



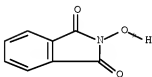
A



F

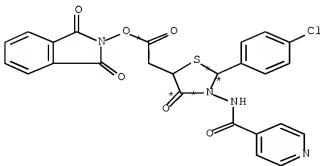


T



AO

4
STEPS
→



AS
 YIELD 68%

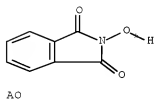
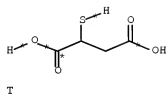
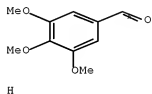
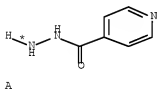
RX(2) RCT A 54-85-3, F 104-88-1
 RGT D 64-19-7 AcOH
 PRO G 6342-46-7
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(10) RCT G 6342-46-7, T 70-49-5
 PRO X 103710-50-5
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 8 hours, reflux

RX(18) RCT X 103710-50-5
 RGT AF 7719-09-7 SOCl2
 PRO AH 890848-60-9
 SOL 71-43-2 Benzene
 CON 60 minutes, reflux

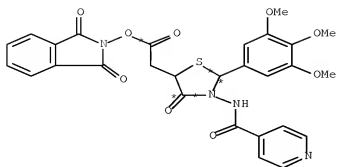
RX(26) RCT AH 890848-60-9, AO 524-38-9
 RGT AQ 121-44-8 Et3N
 PRO AS 890848-68-7
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 3 hours, reflux

RX(70) OF 80 COMPOSED OF RX(3), RX(11), RX(19), RX(27)
 RX(70) A + H + T + AO ==> AT



4
 STEPS
 →

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AT
YIELD 70%

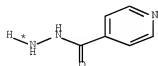
RX(3) RCT A 54-35-3, H 86-81-7
RGT D 64-19-7 AcOH
PRO I 67837-40-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(11) RCT I 67837-40-5, T 70-49-5
PRO Y 890848-58-5
CAT 76,46-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

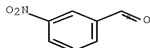
RX(19) RCT Y 890848-58-5
RGT AF 7719-09-7 SOCl2
PRO AI 890848-61-0
SOL 71-43-2 Benzene
CON 60 minutes, reflux

RX(27) RCT AI 890848-61-0, AO 524-38-9
RGT AQ 121-44-8 Et3N
PRO AT 890848-69-3
SOL 68-12-2 DMF
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 3 hours, reflux

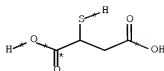
RX(72) OF 80 COMPOSED OF RX(4), RX(12), RX(20), RX(28)
RX(72) A + J + T + AO ==> AU



A

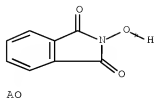


J

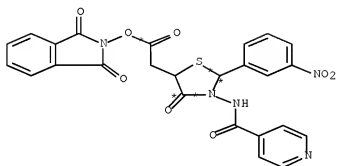


T

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4
STEPS
→



YIELD 63%

RX(4) RCT A 54-85-3, J 99-61-6
RGT D 64-19-7 AcOH
PRO K 16012-26-3
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(12) RCT K 16012-26-3, T 70-45-5
PRO Z 103706-31-6
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

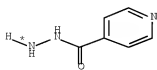
RX(20) RCT Z 103706-31-6
RGT AF 7719-09-7 SOCl2
PRO AJ 890848-62-1
SOL 71-43-2 Benzene
CON 60 minutes, reflux

RX(28) RCT AJ 890848-62-1, AO 524-38-9
RGT AQ 121-44-8 Et3N
PRO AU 890848-70-1
SOL 68-12-2 DMF
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 3 hours, reflux

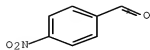
10/595943

RX(74) OF 80 COMPOSED OF RX(5), RX(13), RX(21), RX(29)

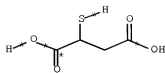
RX(74) A + L + T + AO ==> AV



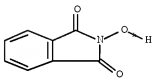
A



L

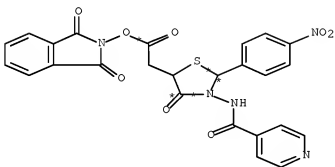


T



AO

4
STEPS
→



AV
YIELD 60%

RX(5) RCT A 54-95-3, L 555-16-8
RGT D 64-19-7 AcOH
PRO M 4813-07-4
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(13) RCT M 4813-07-4, T 70-49-5
PRO AA 103706-32-7
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

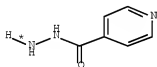
10/595943

RX(21) RCT AA 103706-32-7
 RGT AF 7719-09-7 SOC12
 PRO AK 890848-63-2
 SOL 71-43-2 Benzene
 CON 60 minutes, reflux

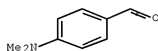
RX(29) RCT AK 890848-63-2, AO 524-38-9
 RGT AQ 121-44-8 Et3N
 PRO AV 890848-71-2
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 3 hours, reflux

RX(76) OF 80 COMPOSED OF RX(6), RX(14), RX(22), RX(30)

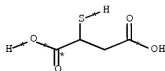
RX(76) A + N + T + AO ==> AW



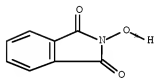
A



N

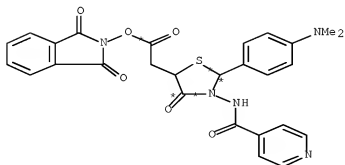


T



AO

4
STEPS
→



AW
YIELD 59%

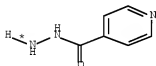
RX(6) RCT A 54-85-3, N 100-10-7
 RGT D 64-19-7 AcOH
 PRO O 13059-77-3
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(14) RCT O 13059-77-3, T 70-49-5
 PRO AB 93607-15-9
 CAT 7646-85-7 ZnCl2
 SOL 109-99-9 THF
 CON 8 hours, reflux

RX(22) RCT AB 93607-15-9
 RGT AF 7719-09-7 SOCl2
 PRO AL 890848-64-3
 SOL 71-43-2 Benzene
 CON 60 minutes, reflux

RX(30) RCT AL 890848-64-3, AO 524-38-9
 RGT AQ 121-44-8 Et3N
 PRO AW 890848-72-3
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 3 hours, reflux

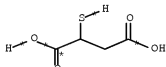
RX(78) OF 80 COMPOSED OF RX(7), RX(15), RX(23), RX(31)
 RX(78) A + P + T + AO ==> AX



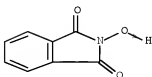
A



P



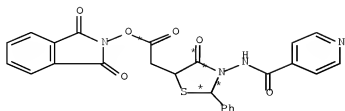
T



AO

4
STEPS
→

10/595943



AX
YIELD 65%

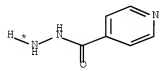
RX(7) RCT A 54-85-3, P 100-52-7
RGT D 64-19-7 AcOH
PRO Q 533-02-8
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(15) RCT Q 533-02-8, T 70-49-5
PRO AC 24327-74-0
CAT 7646-85-7 ZnCl2
SOL 109-99-9 THF
CON 8 hours, reflux

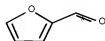
RX(23) RCT AC 24327-74-0
RGT AF 7719-09-7 SOCl2
PRO AM 890848-65-4
SOL 71-43-2 Benzene
CON 60 minutes, reflux

RX(31) RCT AM 890848-65-4, AO 524-38-9
RGT AQ 121-44-8 Et3N
PRO AX 890848-73-4
SOL 68-12-2 DMF
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 3 hours, reflux

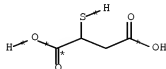
RX(80) OF 80 COMPOSED OF RX(8), RX(16), RX(24), RX(32)
RX(80) A + R + T + AO ==> AY



A

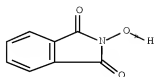


R



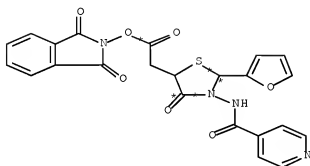
T

10/595943



AO

4
STEPS
→



AY
YIELD 74%

```

RX(8)      RCT  A 54-85-3, R 98-01-1
           RGT  D 64-19-7 AcOH
           PRO  S 6956-53-2
           SOL  64-17-5 EtOH
           CON  4 hours, reflux

RX(16)     RCT  S 6956-53-2, T 70-49-5
           PRO  AD 103706-42-9
           CAT  7646-85-7 ZnCl2
           SOL  109-99-9 THF
           CON  8 hours, reflux

RX(24)     RCT  AD 103706-42-9
           RGT  AF 7719-09-7 SOCl2
           PRO  AN 890848-66-5
           SOL  71-43-2 Benzene
           CON  60 minutes, reflux

RX(32)     RCT  AN 890848-66-5, AO 524-38-9
           RGT  AQ 121-44-8 Et3N
           PRO  AY 890848-74-5
           SOL  68-12-2 DMF
           CON  SUBSTAGE(1) 1 hour, room temperature
                SUBSTAGE(2) room temperature -> reflux
                SUBSTAGE(3) 3 hours, reflux
  
```

10/595943

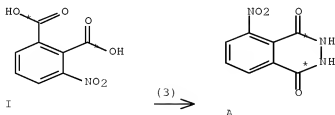
ACCESSION NUMBER: 143:26622 CASREACT Full-text
 TITLE: Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids
 INVENTOR(S): Lopes, Claudio Cerqueira; Lopes, Rosangela Sabattini Capella; Cardoso, Jari Nobrega; Alves Da Silva, Jacqueline; Ferreira Gomes, Leticia
 PATENT ASSIGNEE(S): Universidade Federal do Rio de Janeiro-UFRJ, Brazil
 SOURCE: PCT Int. Appl., 14 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051870	A2	20050609	WO 2004-BR236	20041125
WO 2005051870	A3	20050707		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG BR 2003007864 A 20050705 BR 2003-7864 20031125 US 20070128680 A1 20070607 US 2006-595943 20060522 PRIORITY APPLN. INFO.: BR 2003-7864 20031125 WO 2004-BR236 20041125				

OTHER SOURCE(S): MARPAT 143:26622

AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.

RX(3) OF 6 ...I ==> A...



10/595943

RX(3) RCT I 603-11-2

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

SUBSTAGE(2) 4 hours, 50 deg C

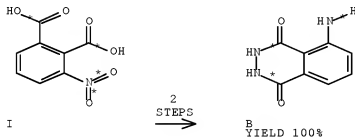
SUBSTAGE(3) cooled

PRO A 3682-15-3

NTE inert

RX(5) OF 6 COMPOSED OF RX(3), RX(1)

RX(5) I ==> B



RX(3) RCT I 603-11-2

STAGE(1)

CAT 10026-12-7 NbCl5

CON 30 minutes, room temperature

STAGE(2)

RGT L 302-01-2 N2H4

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 minutes, room temperature -> 50 deg C

SUBSTAGE(2) 4 hours, 50 deg C

SUBSTAGE(3) cooled

PRO A 3682-15-3

NTE inert

RX(1) RCT A 3682-15-3

RGT C 1333-74-0 H2

PRO B 521-31-3

CAT 7440-05-3 Pd

SOL 123-91-1 Dioxane, 7732-18-5 Water, 64-19-7 AcOH

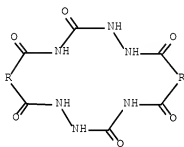
CON room temperature

NTE Pd supported on carbon was used as catalyst, sodium dithionite in acidic medium can also be used as reducing agent

- TI Hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids
- AB A process to form hydrazides (e.g., luminol) from the reaction of a hydrazine and a dicarboxylic (e.g., 3-nitrophthalic acid) using a Lewis acid catalyst (e.g., niobium pentachloride) is described. The reaction occurs in a safe reactional environment, utilizing smooth conditions, neither involving high temps. nor high pressures, producing the desired products with high yields, between 90-95%. The invention also describes a kit for utilization of chemiluminescent substances, comprised of two solns.
- IT Amidation
Amidation catalysts
(hydrazidation; hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT Hydrazides
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT Nitration
Reduction
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT Lewis acids
RL: CAT (Catalyst use); USES (Uses)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 7446-70-0, Aluminum chloride, uses 7447-39-4, Cupric chloride, uses 7487-94-7, MercuryII chloride, uses 7550-45-0, Titanium tetrachloride, uses 7637-07-2, Boron trifluoride, uses 7646-79-9, Cobalt chloride (CoCl₂), uses 7646-85-7, Zinc chloride, uses 7647-18-9, Antimony pentachloride 7705-07-9, Titanium trichloride, uses 7705-08-0, Ferric chloride, uses 7718-54-9, Nickel chloride, uses 7758-89-6, Cuprous chloride 7784-34-1, Arsenic trichloride 7786-30-3, Magnesium chloride, uses 7787-47-5, Beryllium chloride 7787-60-2, Bismuth trichloride 7789-48-2, Magnesium bromide 10025-73-7, Chromium trichloride 10025-91-9, Antimony trichloride 10026-07-0, Tellurium tetrachloride 10026-10-5, Uranium tetrachloride 10026-11-6, Zirconium tetrachloride 10026-12-7, Niobium pentachloride 10049-06-6, Titanium dichloride 10108-64-2, Cadmium chloride 10294-34-5, Boron trichloride 13450-90-3, Gallium chloride 22441-45-8, Arsenic pentachloride
RL: CAT (Catalyst use); USES (Uses)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT 7697-37-2, Nitric acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids)
- IT 85-44-9, Phthalic anhydride
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 603-11-2P, 3-Nitrophthalic acid 3682-15-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 521-31-3P, Luminol
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrazide catalytic production process from hydrazines and dicarboxylic acids in the presence of Lewis acids using)
- IT 67-64-1, Acetone, uses 67-68-5, DmsO, uses 68-12-2, Dmf, uses

123-91-1, Dioxane, uses 872-50-4, NMP, uses
 RL: NUU (Other use, unclassified); USES (Uses)
 (solvent; hydrazide catalytic production process from hydrazines and
 dicarboxylic acids in the presence of Lewis acids
 using)

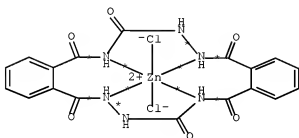
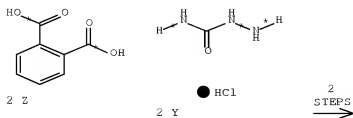
L91 ANSWER 6 OF 30 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 142:474748 CASREACT Full-text
 TITLE: Novel 16-membered [N6] macrocycles bearing hexaamide
 functions and their metal-encapsulated compounds
 AUTHOR(S): Siddiqi, Zafar Ahmad; Shadab, Shah Mohammad
 CORPORATE SOURCE: Division of Inorganic Chemistry, Chemistry Department,
 Aligarh Muslim University, Aligarh, 202002, India
 SOURCE: Indian Journal of Chemistry, Section A: Inorganic,
 Bio-inorganic, Physical, Theoretical & Analytical
 Chemistry (2004), 43A(11), 2274-2280
 CODEN: ICACEC; ISSN: 0376-4710
 PUBLISHER: National Institute of Science Communication
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Cyclocondensation reaction between phthalic anhydride/phthalic acid or succinic anhydride/succinic acid and semicarbazide hydrochloride in DMF-MeOH under reflux affords I.xHCl (R = o-C6H4, x = 0; R = CH2CH2, x = 2). Reactions of the macrocycles with [ML]Cl2 or [M(PPh3)2Cl2] (M = Zn, Cd or Hg) gave MLC12 (L = I). Physicochem. and spectroscopic studies of complexes reveal that proton at aza group (NH) of the amide/peptide function does not deprotonate prior to coordination and hexacoordination around metal ions is maintained.
 REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(23) OF 40 COMPOSED OF RX(14), RX(1)
 RX(23) 2 Z + 2 Y ==> B

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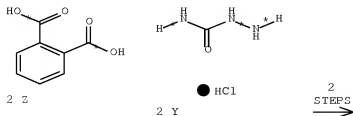


B
YIELD 23%

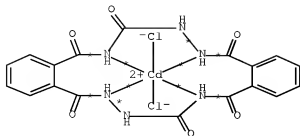
RX(14) RCT Z 88-99-3, Y 563-41-7
 PRO A 851625-90-6
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 6 hours, reflux

RX(1) RCT A 851625-90-6
 RGT C 7646-85-7 ZnCl2
 PRO B 851625-78-0
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 24 hours, room temperature

RX(25) OF 40 COMPOSED OF RX(14), RX(5)
 RX(25) 2 Z + 2 Y ==> L



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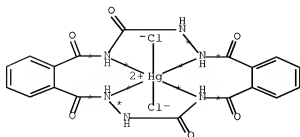
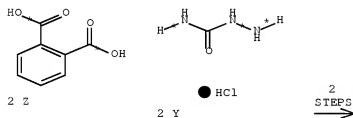


L
YIELD 42%

RX(14) RCT Z 88-99-3, Y 563-41-7
PRO A 851625-90-6
SOL 67-56-1 MeOH, 68-12-2 DMF
CON 6 hours, reflux

RX(5) RCT A 851625-90-6
RGT M 10108-64-2 CdCl2
PRO L 851625-82-6
SOL 67-56-1 MeOH, 68-12-2 DMF
CON 24 hours, room temperature

RX(27) OF 40 COMPOSED OF RX(14), RX(9)
RX(27) 2 Z + 2 Y ==> R

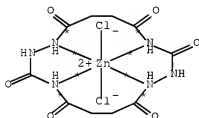
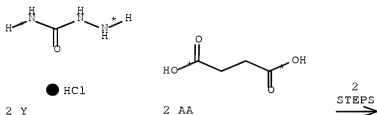


R
YIELD 36%

RX(14) RCT Z 88-99-3, Y 563-41-7
 PRO A 851625-90-6
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 6 hours, reflux

RX(9) RCT A 851625-90-6
 RGT S 7487-94-7 HgCl2
 PRO R 851625-86-0
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 24 hours, room temperature

RX(29) OF 40 COMPOSED OF RX(15), RX(3)
 RX(29) 2 Y + 2 AA ==> J



J
 YIELD 22%

RX(15) RCT Y 563-41-7
 STAGE(1)
 RGT AB 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 1 hour, room temperature

STAGE(2)
 RCT AA 110-15-6
 SOL 123-91-1 Dioxane
 CON SUBSTAGE(1) 6 hours, reflux

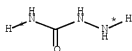
10/595943

SUBSTAGE(2) overnight, room temperature

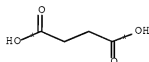
PRO I 851625-91-7

RX(3) RCT I 851625-91-7
 RGT C 7646-85-7 ZnCl2
 PRO J 851625-80-4
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 24 hours, room temperature

RX(31) OF 40 COMPOSED OF RX(15), RX(7)
 RX(31) 2 Y + 2 AA ==> P

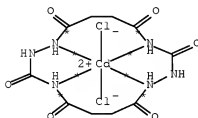


2 Y ● HCl



2 AA

2
STEPS
→



P
YIELD 92%

RX(15) RCT Y 563-41-7

STAGE(1)

RGT AB 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 1 hour, room temperature

STAGE(2)

RCT AA 110-15-6
 SOL 123-91-1 Dioxane
 CON SUBSTAGE(1) 6 hours, reflux
 SUBSTAGE(2) overnight, room temperature

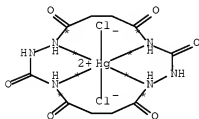
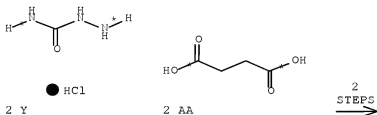
PRO I 851625-91-7

RX(7) RCT I 851625-91-7

10/595943

RGT M 10108-64-2 CdCl2
 PRO P 851625-84-3
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 24 hours, room temperature

RX(33) OF 40 COMPOSED OF RX(15), RX(11)
 RX(33) 2 Y + 2 AA ==> V



V
 YIELD 89%

RX(15) RCT Y 563-41-7

STAGE(1)

RGT AB 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 1 hour, room temperature

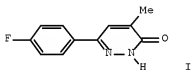
STAGE(2)

RCT AA 110-15-6
 SOL 123-91-1 Dioxane
 CON SUBSTAGE(1) 6 hours, reflux
 SUBSTAGE(2) overnight, room temperature

PRO I 851625-91-7

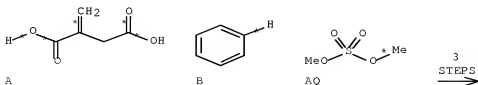
RX(11) RCT I 851625-91-7
 RGT S 7487-94-7 HgCl2
 PRO V 851625-88-2
 SOL 67-56-1 MeOH, 68-12-2 DMF
 CON 24 hours, room temperature

L91 ANSWER 7 OF 30 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 142:261502 CASREACT Full-text
 TITLE: Synthesis and hypotensive activity of some
 6-(substituted
 aryl)-4-methyl-2,3-dihydropyridazin-3-ones
 AUTHOR(S): Siddiqui, Anees A.; Wani, Sachin M.
 CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of
 Pharmacy, Hamdard University, New Delhi, 110 062,
 India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (2004),
 43B(7), 1574-1579
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

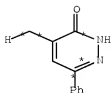


AB 6-Aryl-4-methyl-2,3-dihydropyridazin-3-ones, e.g., I, were synthesized by cyclization of appropriate β -aroyl-2-methylene propionate with hydrazine hydrate in the presence of sodium acetate. The title compds. were tested for hypotensive activity, non-invasively, by tail-cuff method and were found to possess significant hypotensive activity in normotensive rats.
 REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(101) OF 120 COMPOSED OF RX(1), RX(21), RX(41)
 RX(101) A + B + AQ ==> BN



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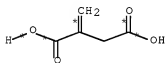
BN
YIELD 65%

RX(1) RCT A 97-65-4, B 71-43-2
RGT D 7446-70-0 AlCl3
PRO C 15732-75-9
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

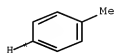
RX(21) RCT C 15732-75-9, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO AR 148903-67-7
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(41) RCT AR 148903-67-7
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BN 13300-09-9
SOL 67-56-1 MeOH
CON 8 hours, reflux

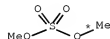
RX(102) OF 120 COMPOSED OF RX(2), RX(22), RX(42)
RX(102) A + E + AQ ==> BK



A

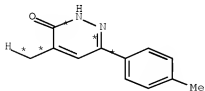


E



AQ

3
STEPS
→



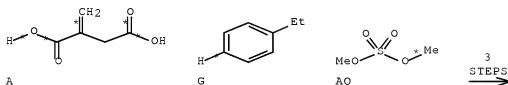
BR
YIELD 80%

RX(2) RCT A 97-65-4, E 108-88-3
 RGT D 7446-70-0 AlCl3
 PRO F 19340-33-1
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) reflux
 SUBSTAGE(2) 4 hours, reflux

RX(22) RCT F 19340-33-1, AQ 77-78-1
 RGT AS 584-08-7 K2CO3
 PRO AU 845961-24-2
 SOL 75-05-8 MeCN
 CON 4 hours, reflux

RX(42) RCT AU 845961-24-2
 RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
 PRO BR 21004-61-5
 SOL 67-56-1 MeOH
 CON 8 hours, reflux

RX(103) OF 120 COMPOSED OF RX(3), RX(23), RX(43)
 RX(103) A + G + AQ ==> BS



BS
 YIELD 75%

RX(3) RCT A 97-65-4, G 100-41-4
 RGT D 7446-70-0 AlCl3
 PRO H 118540-59-3
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) reflux
 SUBSTAGE(2) 4 hours, reflux

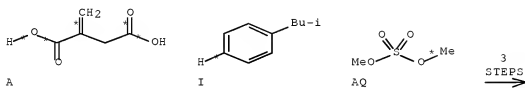
RX(23) RCT H 118540-59-3, AQ 77-78-1
 RGT AS 584-08-7 K2CO3

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PRO AV 845961-25-3
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(43) RCT AV 845961-25-3
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BS 845961-17-3
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(104) OF 120 COMPOSED OF RX(4), RX(24), RX(44)
RX(104) A + I + AQ ==> BT



BT
YIELD 72%

RX(4) RCT A 97-65-4, I 538-93-2
RGT D 7446-70-0 AlCl3
PRO J 845961-43-5
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

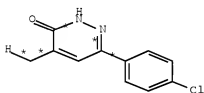
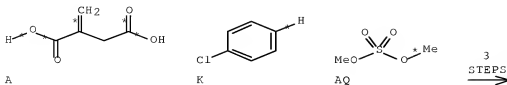
RX(24) RCT J 845961-43-5, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO AW 845961-26-4
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(44) RCT AW 845961-26-4
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BT 845961-18-4
SOL 67-56-1 MeOH
CON 8 hours, reflux

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RX(105) OF 120 COMPOSED OF RX(5), RX(25), RX(45)

RX(105) A + K + AQ ==> BU



BU
YIELD 66%

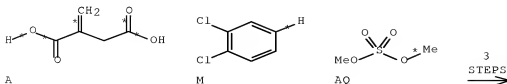
RX(5) RCT A 97-65-4, K 108-90-7
RGT D 7446-70-0 AlCl3
PRO L 58182-59-5
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

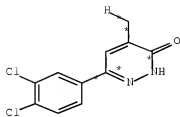
RX(25) RCT L 58182-59-5, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO AX 845961-27-5
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(45) RCT AX 845961-27-5
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BU 32193-12-7
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(106) OF 120 COMPOSED OF RX(6), RX(26), RX(46)

RX(106) A + M + AQ ==> B'





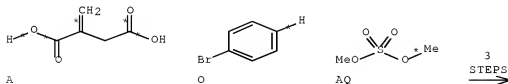
BV
YIELD 65%

RX(6) RCT A 97-65-4, M 95-50-1
RGT D 7446-70-0 AlCl3
PRO N 191018-61-8
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

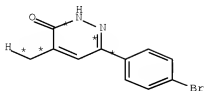
RX(26) RCT N 191018-61-8, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO AY 845961-28-6
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(46) RCT AY 845961-28-6
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BV 845961-19-5
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(107) OF 120 COMPOSED OF RX(7), RX(27), RX(47)
RX(107) A + O + AQ ==> BV



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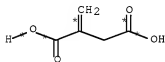
BW
YIELD 68%

RX(7) RCT A 97-65-4, O 108-86-1
RGT D 7446-70-0 AlCl3
PRO P 101973-98-2
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

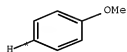
RX(27) RCT P 101973-98-2, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO AZ 845961-29-7
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(47) RCT AZ 845961-29-7
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BW 21004-64-8
SOL 67-56-1 MeOH
CON 8 hours, reflux

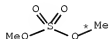
RX(108) OF 120 COMPOSED OF RX(8), RX(28), RX(48)
RX(108) A + Q + AQ ==> BX



A

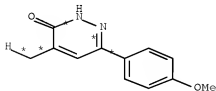


Q



AQ

3
STEPS
→



BX
YIELD 75%

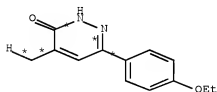
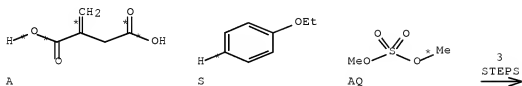
RX(8) RCT A 97-65-4, Q 100-66-3
 RGT D 7446-70-0 AlCl3
 PRO R 101973-94-8
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) reflux
 SUBSTAGE(2) 4 hours, reflux

 RX(28) RCT R 101973-94-8, AQ 77-78-1
 RGT AS 584-08-7 K2CO3
 PRO BA 845961-30-0
 SOL 75-05-8 MeCN
 CON 4 hours, reflux

 RX(48) RCT BA 845961-30-0
 RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
 PRO BX 28657-53-6
 SOL 67-56-1 MeOH
 CON 8 hours, reflux

RX(109) OF 120 COMPOSED OF RX(9), RX(29), RX(49)

RX(109) A + S + AQ ==> BY



YIELD 72%

RX(9) RCT A 97-65-4, S 103-73-1
 RGT D 7446-70-0 AlCl3
 PRO T 845961-44-6
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) reflux
 SUBSTAGE(2) 4 hours, reflux

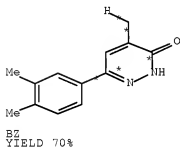
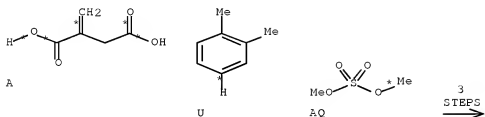
RX(29) RCT T 845961-44-6, AQ 77-78-1
 RGT AS 584-08-7 K2CO3

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PRO BB 845961-31-1
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(49) RCT BB 845961-31-1
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO BY 845961-20-8
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(110) OF 120 COMPOSED OF RX(10), RX(30), RX(50)
RX(110) A + U + AQ ==> BZ



RX(10) RCT A 97-65-4, U 95-47-6
RGT D 7446-70-0 AlCl3
PRO V 101973-97-1
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

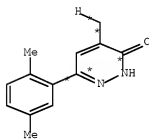
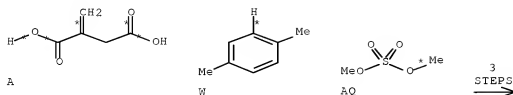
RX(30) RCT V 101973-97-1, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BC 845961-32-2
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(50) RCT BC 845961-32-2
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4

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PRO BZ 64262-76-6
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(111) OF 120 COMPOSED OF RX(11), RX(31), RX(51)
RX(111) A + W + AQ ==> CA



CA
YIELD 66%

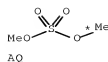
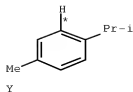
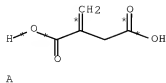
RX(11) RCT A 97-65-4, W 106-42-3
RGT D 7446-70-0 AlCl3
PRO X 118540-58-2
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

RX(31) RCT X 118540-58-2, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BD 845961-33-3
SOL 75-05-8 MeCN
CON 4 hours, reflux

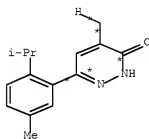
RX(51) RCT BD 845961-33-3
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CA 64262-78-8
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(112) OF 120 COMPOSED OF RX(12), RX(32), RX(52)
RX(112) A + Y + AQ ==> CB

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3
STEPS
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CB
YIELD 70%

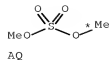
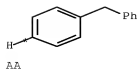
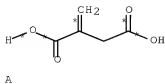
RX(12) RCT A 37-65-4, Y 99-87-6
RGT D 7446-70-0 AlCl3
PRO Z 845961-45-7
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

RX(32) RCT Z 845961-45-7, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BE 845961-34-4
SOL 75-05-8 MeCN
CON 4 hours, reflux

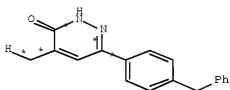
RX(52) RCT BE 845961-34-4
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CB 845961-21-5
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(113) OF 120 COMPOSED OF RX(13), RX(33), RX(53)
RX(113) A + AA + AQ ==> CC

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3
STEPS
→



YIELD 66%

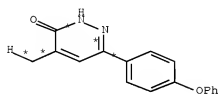
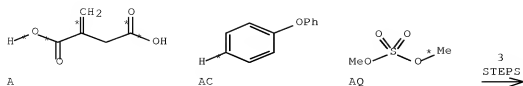
RX(13) RCT A 97-65-4, AA 101-81-5
RGT D 7446-70-0 AlCl3
PRO AB 845961-46-8
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

RX(33) RCT AB 845961-46-8, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BF 845961-35-5
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(53) RCT BF 845961-35-5
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CC 845961-22-0
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(114) OF 120 COMPOSED OF RX(14), RX(34), RX(54)
RX(114) A + AC + AQ ==> CC

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CD
YIELD 71%

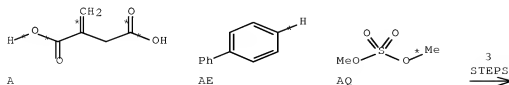
RX(14) RCT A 97-65-4, AC 101-84-8
RGT D 7446-73-0 AlCl3
PRO AD 58182-60-8
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

RX(34) RCT AD 58182-60-8, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BG 845961-36-6
SOL 75-05-8 MeCN
CON 4 hours, reflux

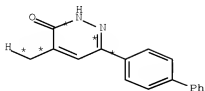
RX(54) RCT BG 845961-36-6
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CD 68195-42-6
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(115) OF 120 COMPOSED OF RX(15), RX(35), RX(55)

RX(115) A + AE + AQ ==> CE



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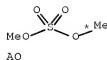
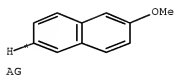
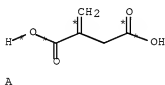
CE
YIELD 76%

RX(15) RCT A 97-65-4, AE 92-52-4
RGT D 7446-70-0 AlCl3
PRO AF 19340-35-3
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

RX(35) RCT AF 19340-35-3, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BH 845961-37-7
SOL 75-05-8 MeCN
CON 4 hours, reflux

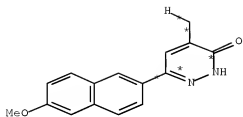
RX(55) RCT BH 845961-37-7
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CE 21004-63-7
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(116) OF 120 COMPOSED OF RX(16), RX(36), RX(56)
RX(116) A + AG + AQ ==> CF



3
STEPS
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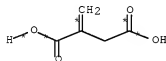
CF
YIELD 57%

RX(16) RCT A 97-65-4, AG 93-04-9
RGT D 7446-70-0 AlCl3
PRO AH 845961-47-9
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

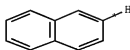
RX(36) RCT AH 845961-47-9, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BI 845961-38-8
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(56) RCT BI 845961-38-8
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CF 845961-23-1
SOL 67-56-1 MeOH
CON 8 hours, reflux

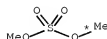
RX(117) OF 120 COMPOSED OF RX(17), RX(37), RX(57)
RX(117) A + AI + AQ ==> CG



A



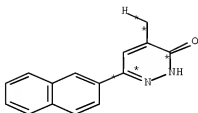
AI



AQ

3
STEPS
→

10/595943



CG
YIELD 54%

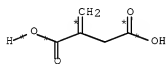
RX(17) RCT A 97-65-4, AI 91-20-3
RGT D 7446-79-0 AlCl3
PRO AJ 60186-01-8
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

RX(37) RCT AJ 60186-01-8, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BJ 845961-39-9
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(57) RCT BJ 845961-39-9
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CG 28734-27-2
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(118) OF 120 COMPOSED OF RX(18), RX(38), RX(58)

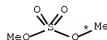
RX(118) A + AK + AQ ==> CH



A

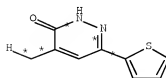


AK



AQ

3
STEPS
→



CH
YIELD 56%

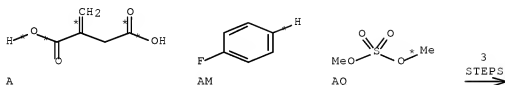
RX(18) RCT A 97-65-4, AK 110-02-1
 RGT D 7446-70-0 AlCl3
 PRO AL 845961-48-0
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) reflux
 SUBSTAGE(2) 4 hours, reflux

 RX(38) RCT AL 845961-48-0, AQ 77-78-1
 RGT AS 584-08-7 K2CO3
 PRO BK 845961-40-2
 SOL 75-05-8 MeCN
 CON 4 hours, reflux

 RX(58) RCT BK 845961-40-2
 RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
 PRO CH 28657-57-0
 SOL 67-56-1 MeOH
 CON 8 hours, reflux

RX(119) OF 120 COMPOSED OF RX(19), RX(39), RX(59)

RX(119) A + AM + AQ ==> CI



CI
YIELD 62%

RX(19) RCT A 97-65-4, AM 462-06-6
 RGT D 7446-70-0 AlCl3
 PRO AN 58182-61-9
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) reflux
 SUBSTAGE(2) 4 hours, reflux

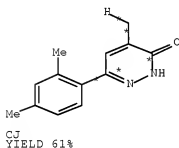
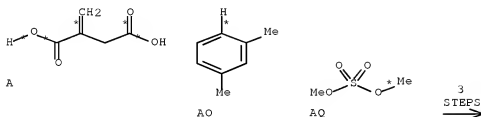
RX(39) RCT AN 58182-61-9, AQ 77-78-1
 RGT AS 584-08-7 K2CO3

10/595943

PRO BL 845961-41-3
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(59) RCT BL 845961-41-3
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4
PRO CI 68612-32-8
SOL 67-56-1 MeOH
CON 8 hours, reflux

RX(120) OF 120 COMPOSED OF RX(20), RX(40), RX(60)
RX(120) A + AO + AQ ==> CJ



RX(20) RCT A 57-65-4, AO 108-38-3
RGT D 7446-70-0 AlCl3
PRO AP 101973-96-0
SOL 71-43-2 Benzene
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 4 hours, reflux

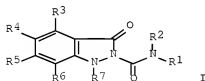
RX(40) RCT AP 101973-96-0, AQ 77-78-1
RGT AS 584-08-7 K2CO3
PRO BM 845961-42-4
SOL 75-05-8 MeCN
CON 4 hours, reflux

RX(60) RCT BM 845961-42-4
RGT BO 127-09-3 AcONa, BP 302-01-2 N2H4

PRO CJ 64262-77-7
 SOL 67-56-1 MeOH
 CON 8 hours, reflux

L91 ANSWER 8 OF 30 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 141:395549 CASREACT Full-text
 TITLE: Preparation of 3-oxo-1,3-dihydro-indazole-2-carboxylic acid amide derivatives as phospholipase inhibitors
 INVENTOR(S): Eacho, Patrick Irving; Foxworthy-Mason, Patricia Sue; Lin, Ho-Shen; Lopez, Jose Eduardo; Mosior, Marian Kazimierz; Richett, Michael Enrico
 PATENT ASSIGNEE(S): Eli Lilly and Company, USA
 SOURCE: PCT Int. Appl., 131 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004093872	A1	20041104	WO 2004-US6092	20040325
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1610779	A1	20060104	EP 2004-723448	20040325
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK			
US 20060211755	A1	20060921	US 2005-544910	20050810
PRIORITY APPLN. INFO.:			US 2003-459362P	20030331
			WO 2004-US6092	20040325
OTHER SOURCE(S):	MARPAT 141:395549			
GI				



AB Title compds. I [R1 = alkyl, haloalkyl, alkenyl, alkynyl, etc.; R2 = H; R3-6 = H, alk(en/yn)yl, haloalkyl, etc.; R7 = H, alk(en/yn)yl, haloalkyl, etc.] are prepared For instance, 3-oxo-1,3-dihydroindazole-2-carboxylic acid N-propylamide is prepared from Pr isocyanate and 1,2-dihydroindazol-3-one.

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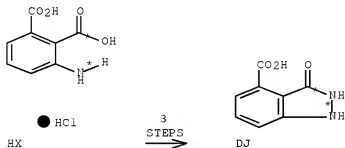
Selected compds. exhibited inhibitory activity toward endothelial lipase; IC50 11.39 - 45.14 nM. I are useful for the treatment of hepatic lipase and/or endothelial lipase-mediated diseases.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

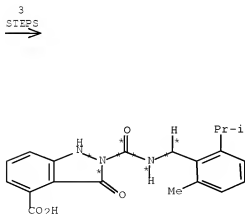
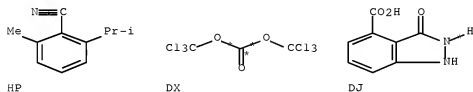
RX(365) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(65)
AND REACTION SEQUENCE RX(107), RX(121), RX(65)

... WX ==> DJ...

...HP + DX + DJ ==> EP



START NEXT REACTION SEQUENCE



EP
YIELD 69%

RX(115) RCT HX 6946-20-1

STAGE(1)

RGT DP 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 10 minutes, -10 deg C

STAGE(2)

RGT DQ 7632-00-0 NaNO2
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) -10 deg C
 SUBSTAGE(2) 1 hour, -10 deg C

STAGE(3)

RGT DP 7647-01-0 HCl, DR 7772-99-8 SnCl2
 SOL 7732-18-5 Water, 7647-01-0 HCl
 CON SUBSTAGE(1) 15 minutes, -10 deg C
 SUBSTAGE(2) 30 minutes, -10 deg C
 SUBSTAGE(3) -10 deg C -> room temperature
 SUBSTAGE(4) 16 hours, room temperature

PRO DJ 7384-17-0

NTE incremental addition of the diazotized solution in third stage

RX(107) RCT HP 786677-15-4

STAGE(1)

RGT BS 16940-66-2 NaBH4
 SOL 60-29-7 Et2O
 CON SUBSTAGE(1) 16 hours, room temperature
 SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT BV 67-56-1 MeOH
 CON 0 deg C

PRO BX 786677-17-6

RX(121) RCT BX 786677-17-6, DX 32315-10-9

RGT EA 20734-58-1 Proton sponge
 PRO EO 787580-99-8
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 15 minutes, room temperature

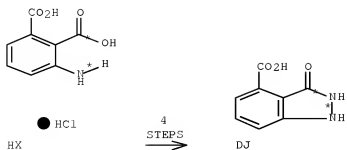
RX(65) RCT DJ 7384-17-0, EO 787580-99-8

PRO EP 787580-05-6
 SOL 109-99-9 THF
 CON 16 hours, room temperature
 NTE chemoselective

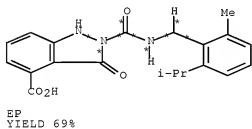
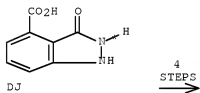
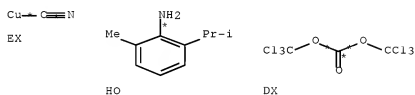
RX(419) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(65)
 AND REACTION SEQUENCE RX(106), RX(107), RX(121), RX(65)

... HX ==> DJ...
 ...EX + HO + DX + DJ ==> EP

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START NEXT REACTION SEQUENCE



RX(115) RCT HX 6346-22-1

STAGE(1)

RGT DP 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 10 minutes, -10 deg C

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STAGE(2)
  RGT  DQ 7632-00-0 NaNO2
  SOL  7732-18-5 Water
  CON  SUBSTAGE(1) -10 deg C
        SUBSTAGE(2) 1 hour, -10 deg C

STAGE(3)
  RGT  DP 7647-01-0 HCl, DR 7732-99-8 SnCl2
  SOL  7732-18-5 Water, 7647-01-0 HCl
  CON  SUBSTAGE(1) 15 minutes, -10 deg C
        SUBSTAGE(2) 30 minutes, -10 deg C
        SUBSTAGE(3) -10 deg C -> room temperature
        SUBSTAGE(4) 16 hours, room temperature

PRO   DJ 7384-17-0
NTE   incremental addition of the diazotized solution in third stage

RX(106) RCT  EX 544-92-3

STAGE(1)
  RGT  FA 594-70-7 Propane, 2-methyl-2-nitro-
  SOL  67-68-5 DMSO
  CON  60 deg C

STAGE(2)
  RCT  HO 5266-85-3
  SOL  67-68-5 DMSO
  CON  SUBSTAGE(1) 60 deg C
        SUBSTAGE(2) 1 hour, 60 deg C
        SUBSTAGE(3) 60 deg C -> 45 deg C

STAGE(3)
  RGT  DP 7647-01-0 HCl
  SOL  7732-18-5 Water
  CON  SUBSTAGE(1) 5 minutes, 45 deg C
        SUBSTAGE(2) 45 deg C -> room temperature

PRO   HP 786677-15-4

RX(107) RCT  HP 786677-15-4

STAGE(1)
  RGT  BS 16940-66-2 NaBH4
  SOL  60-29-7 Et2O
  CON  SUBSTAGE(1) 16 hours, room temperature
        SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
  RGT  BV 67-56-1 MeOH
  CON  0 deg C

PRO   BX 786677-17-6

RX(121) RCT  BX 786677-17-6, DX 32315-10-9
  RGT  EA 20734-58-1 Proton sponge
  PRO  EO 787580-99-8
  SOL  75-09-2 CH2Cl2
  CON  SUBSTAGE(1) 0 deg C
        SUBSTAGE(2) 15 minutes, room temperature

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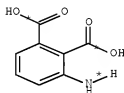
10/595943

RX(65) RCT DJ 7384-17-0, EO 787580-99-8
 PRO EP 787580-05-6
 SOL 109-99-9 THF
 CON 16 hours, room temperature
 NTE chemoselective

RX(436) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(142), RX(101)
 AND REACTION SEQUENCE RX(107), RX(121), RX(101)

...HX + BV ==> HE...

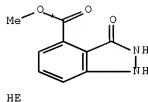
...HP + DX + HE ==> HK



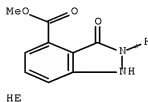
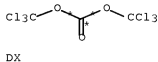
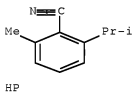
HX
 ● HCl



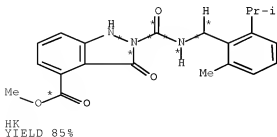
3
 STEPS
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START NEXT REACTION SEQUENCE



3
 STEPS
 →



```

RX(115)  RCT  HX 6346-22-1

          STAGE(1)
          RGT  DP 7647-01-0 HCl
          SOL  7732-18-5 Water
          CON  10 minutes, -10 deg C

          STAGE(2)
          RGT  DQ 7632-00-0 NaNO2
          SOL  7732-18-5 Water
          CON  SUBSTAGE(1) -10 deg C
              SUBSTAGE(2) 1 hour, -10 deg C

          STAGE(3)
          RGT  DP 7647-01-0 HCl, DR 7772-99-8 SnCl2
          SOL  7732-18-5 Water, 7647-01-0 HCl
          CON  SUBSTAGE(1) 15 minutes, -10 deg C
              SUBSTAGE(2) 30 minutes, -10 deg C
              SUBSTAGE(3) -10 deg C -> room temperature
              SUBSTAGE(4) 16 hours, room temperature

          PRO  DJ 7384-17-0
          NTE  incremental addition of the diazotized solution in third stage

RX(142)  RCT  DJ 7384-17-0, BV 67-56-1
          RGT  DP 7647-01-0 HCl
          PRO  HE 787581-35-5
          SOL  7732-18-5 Water, 67-56-1 MeOH
          CON  4 hours, room temperature -> reflux

RX(107)  RCT  HP 786677-15-4

          STAGE(1)
          RGT  BS 16940-66-2 NaBH4
          SOL  60-29-7 Et2O
          CON  SUBSTAGE(1) 16 hours, room temperature
              SUBSTAGE(2) room temperature -> 0 deg C

          STAGE(2)
          RGT  BV 67-56-1 MeOH
          CON  0 deg C

          PRO  BX 786677-17-6

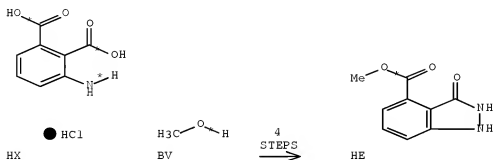
RX(121)  RCT  BX 786677-17-6, DX 32315-10-9
          RGT  EA 20734-58-1 Proton sponge
          PRO  EO 787580-99-8
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) 0 deg C
              SUBSTAGE(2) 15 minutes, room temperature

RX(101)  RCT  EO 787580-99-8, HE 787581-35-5
          PRO  HK 787580-99-8
          SOL  68-12-2 DMF
          CON  3 hours, room temperature

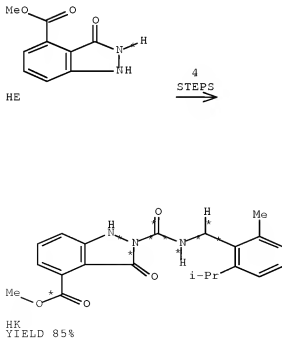
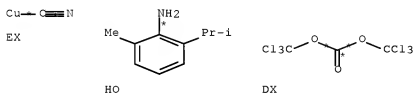
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RX(451) OF 500 COMPOSED OF REACTION SEQUENCE RX(115), RX(142), RX(101)
AND REACTION SEQUENCE RX(106), RX(107), RX(121), RX(101)
... HX + BV ==> HE...
...EX + HO + DX + HE ==> HK



START NEXT REACTION SEQUENCE



RX(115) RCT HX 6346-22-1

STAGE(1)

RGT DP 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 10 minutes, -10 deg C

STAGE(2)

RGT DQ 7632-00-0 NaNO2
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) -10 deg C
 SUBSTAGE(2) 1 hour, -10 deg C

STAGE(3)

RGT DP 7647-01-0 HCl, DR 7772-99-8 SnCl2
 SOL 7732-18-5 Water, 7647-01-0 HCl
 CON SUBSTAGE(1) 15 minutes, -10 deg C
 SUBSTAGE(2) 30 minutes, -10 deg C
 SUBSTAGE(3) -10 deg C -> room temperature
 SUBSTAGE(4) 16 hours, room temperature

PRO DJ 7384-17-0

NTE incremental addition of the diazotized solution in third stage

RX(142) RCT DJ 7384-17-0, BV 67-56-1

RGT DP 7647-01-0 HCl
 PRO HE 787581-35-5
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON 4 hours, room temperature -> reflux

RX(106) RCT EX 544-92-3

STAGE(1)

RGT FA 594-70-7 Propane, 2-methyl-2-nitro-
 SOL 67-68-5 DMSO
 CON 60 deg C

STAGE(2)

RCT HO 5266-85-3
 SOL 67-68-5 DMSO
 CON SUBSTAGE(1) 60 deg C
 SUBSTAGE(2) 1 hour, 60 deg C
 SUBSTAGE(3) 60 deg C -> 45 deg C

STAGE(3)

RGT DP 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 5 minutes, 45 deg C
 SUBSTAGE(2) 45 deg C -> room temperature

PRO HP 786677-15-4

RX(107) RCT HP 786677-15-4

STAGE(1)

RGT BS 16940-66-2 NaBH4

SOL 60-29-7 Et2O
 CON SUBSTAGE(1) 16 hours, room temperature
 SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
 RGT BV 67-56-1 MeOH
 CON 0 deg C

PRO BX 786677-17-6

RX(121) RCT BX 786677-17-6, DX 32315-10-9
 RGT EA 20734-58-1 Proton sponge
 PRO EO 787580-99-8
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 15 minutes, room temperature

RX(101) RCT EO 787580-99-8, HE 787581-35-5
 PRO HK 787580-78-3
 SOL 68-12-2 DMF
 CON 3 hours, room temperature

L91 ANSWER 9 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 141:306350 CASREACT Full-text

TITLE: One- and three-dimensional coordination polymers containing organic ligands produced through in situ hydrothermal reactions

AUTHOR(S): Hu, Xi-Xue; Pan, Cheng-Ling; Xu, Ji-Qing; Cui, Xiao-Bing; Yang, Guang-Di; Wang, Tie-Gang

CORPORATE SOURCE: College of Chemistry and State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, Changchun, 130023, Peop. Rep. China

SOURCE: European Journal of Inorganic Chemistry (2004), (7), 1566-1569

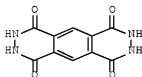
CODEN: EJICFO; ISSN: 1434-1948

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

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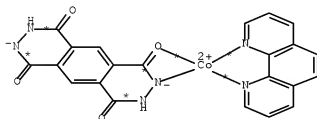
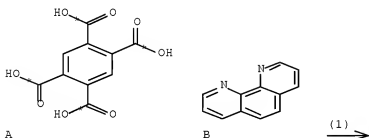
AB Two novel coordination polymers of cobalt(II), [Co(μ 3-H2bbh)(phen)]_n (1) and [Co(μ 4-H2bbh)(H2O)]_{2n} (2, phen = 1,10-phenanthroline; H4bbh = benzene-1,2,4,5-tetracarboxylic dihydrazide, I), in which H2bbh ligands are in situ generated by an acylation reaction of H4bta (H4bta = benzene-1,2,4,5-tetracarboxylic acid) with hydrazine hydrate under hydrothermal conditions, were synthesized and structurally characterized. 1 Has a one-dimensional

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double-chain structure, while 2 has a three-dimensional network structure.
Preliminary magnetic studies of 1 and 2 are reported.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

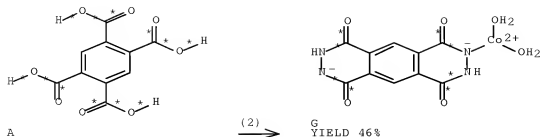
RX(1) OF 2 A + B ==> C



C
YIELD 41%

RX(1) RCT A 89-05-4, B 66-71-7
RGT D 302-01-2 N2H4, E 7646-79-9 CoCl2
PRO C 681439-74-7
SOL 7732-18-5 Water
CON SUBSTAGE(1) 4 days, 170 deg C
SUBSTAGE(2) 170 deg C -> room temperature
NTE thermal, hydrothermal, Teflon-lined stainless steel autoclave
used

RX(2) OF 2 A ==> C



RX(2) RCT A 89-85-4
 RGT D 302-01-2 N2H4, E 7646-79-9 CoCl2
 PRO G 765313-22-2
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 4 days, 170 deg C
 SUBSTAGE(2) 170 deg C -> room temperature
 NTE thermal, hydrothermal, Teflon-lined stainless steel autoclave used

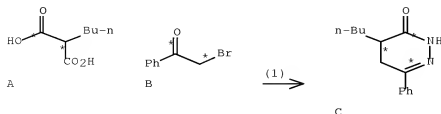
L91 ANSWER 10 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 141:225427 CASREACT [Full-text](#)
 TITLE: Novel and efficient solid-phase synthesis of 4,6-disubstituted 4,5-dihydro-3(2H)-pyridazinone
 AUTHOR(S): Tang, Jing; Huang, Xian
 CORPORATE SOURCE: Dep. Chem., Zhejiang Univ., Hangzhou, 310 028, Peop. Rep. China
 SOURCE: Journal of Chemical Research, Synopses (2003), (9), 599-600
 CODEN: JRPSCD; ISSN: 0308-2342
 PUBLISHER: Science Reviews
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The resin-bound 5-monosubstituted cyclic malonic ester was generated and reacted with an α -bromoketone to give the corresponding 5,5-disubstituted cyclic malonic ester resin. Subsequent reaction with hydrazine resulted in cyclization with concomitant cleavage from the polymeric support to release the final products, 4,6-disubstituted 4,5-dihydro-3(2H)-pyridazinones, in good yield and high purity.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 9 A + B ==> C



RX(1)

STAGE(1)

RGT D 100-44-7D PhCH₂Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
 SOL 68-12-2 DMF
 CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
 SOL 67-68-5 DMSO
 CON 48 hours, 140 deg C

STAGE(3)

RCT A 534-59-8
 RGT G 108-24-7 Ac₂O, H 7664-93-9 H₂SO₄
 SOL 7732-18-5 Water

STAGE(4)

RCT B 70-11-1
 RGT I 127-09-3 AcONa, J 64-19-7 AcOH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) 24 hours, room temperature

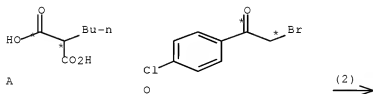
STAGE(5)

RGT K 302-01-2 N₂H₄
 SOL 7732-18-5 Water, 68-12-2 DMF
 CON 17 hours, room temperature

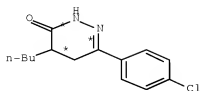
PRO C 746662-97-5

NTE solid-supported reagent, Merrifield resin used

RX(2) OF 9 A + O ==> P



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P

RX(2)

STAGE(1)

RGT D 100-44-7D PhCH2Cl, E 19232-39-4 Butanoic acid, 3-oxo-,
ethyl ester, ion(1-), sodium (1:1)
SOL 68-12-2 DMF
CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
SOL 67-68-5 DMSO
CON 48 hours, 140 deg C

STAGE(3)

RCT A 534-59-8
RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4
SOL 7732-18-5 Water

STAGE(4)

RCT O 536-38-9
RGT I 127-09-3 AcONa, J 64-19-7 AcOH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) 24 hours, room temperature

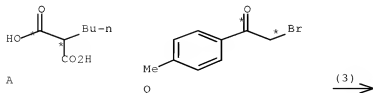
STAGE(5)

RGT K 302-01-2 N2H4
SOL 7732-18-5 Water, 68-12-2 DMF
CON 17 hours, room temperature

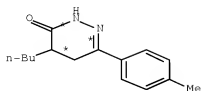
PRO P 746662-98-6

NTE solid-supported reagent, Merrifield resin used

RX(3) OF 9 A + Q ==> R



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R

RX(3)

STAGE(1)

RGT D 100-44-7D PhCH₂Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
 SOL 68-12-2 DMF
 CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
 SOL 67-68-5 DMSO
 CON 48 hours, 140 deg C

STAGE(3)

RCT A 534-59-8
 RGT G 108-24-7 Ac₂O, H 7664-93-9 H₂SO₄
 SOL 7732-18-5 Water

STAGE(4)

RCT Q 619-41-0
 RGT I 127-09-3 AcONa, J 64-19-7 AcOH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) 24 hours, room temperature

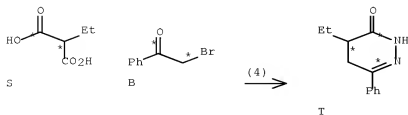
STAGE(5)

RGT K 302-01-2 N₂H₄
 SOL 7732-18-5 Water, 68-12-2 DMF
 CON 17 hours, room temperature

PRO R 746662-99-7

NTE solid-supported reagent, Merrifield resin used

RX(4) OF 9 S + B ==> T



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RX(4)

STAGE(1)

RGT D 100-44-7D PhCH₂Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
 SOL 68-12-2 DMF
 CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
 SOL 67-68-5 DMSO
 CON 48 hours, 140 deg C

STAGE(3)

RCT S 601-75-2
 RGT G 108-24-7 Ac₂O, H 7664-93-9 H₂SO₄
 SOL 7732-18-5 Water

STAGE(4)

RCT B 70-11-1
 RGT I 127-09-3 AcONa, J 64-19-7 AcOH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) 24 hours, room temperature

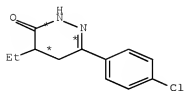
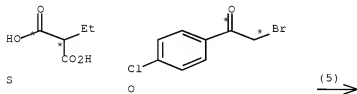
STAGE(5)

RGT K 302-01-2 N₂H₄
 SOL 7732-18-5 Water, 68-12-2 DMF
 CON 17 hours, room temperature

PRO T 24737-96-0

NTE solid-supported reagent, Merrifield resin used

RX(5) OF 9 S + O ==> U



U

RX(5)

STAGE(1)

RGT D 100-44-7D PhCH₂Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
 SOL 68-12-2 DMF
 CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
 SOL 67-68-5 DMSO
 CON 48 hours, 140 deg C

STAGE(3)

RCT S 601-75-2
 RGT G 108-24-7 Ac₂O, H 7664-93-9 H₂SO₄
 SOL 7732-18-5 Water

STAGE(4)

RCT O 536-38-9
 RGT I 127-09-3 AcONa, J 64-19-7 AcOH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) 24 hours, room temperature

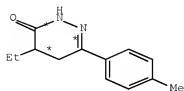
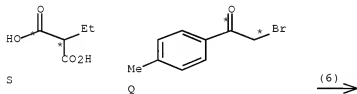
STAGE(5)

RGT K 302-01-2 N₂H₄
 SOL 7732-18-5 Water, 68-12-2 DMF
 CON 17 hours, room temperature

PRO U 746663-00-3

NTE solid-supported reagent, Merrifield resin used

RX(6) OF 9 S + Q ==> V



RX(6)

STAGE(1)

RGT D 100-44-7D PhCH₂Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
 SOL 68-12-2 DMF
 CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
 SOL 67-68-5 DMSO
 CON 48 hours, 140 deg C

STAGE(3)

RCT S 601-75-2
 RGT G 108-24-7 Ac₂O, H 7664-93-9 H₂SO₄
 SOL 7732-18-5 Water

STAGE(4)

RCT Q 619-41-0
 RGT I 127-09-3 AcONa, J 64-19-7 AcOH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) 24 hours, room temperature

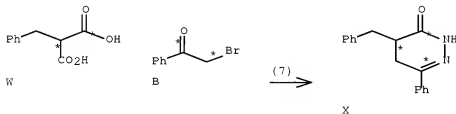
STAGE(5)

RGT K 302-01-2 N₂H₄
 SOL 7732-18-5 Water, 68-12-2 DMF
 CON 17 hours, room temperature

PRO V 24737-97-1

NTE solid-supported reagent, Merrifield resin used

RX(7) OF 9 W + B ==> X



RX(7)

STAGE(1)

RGT D 100-44-7D PhCH₂Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
 SOL 68-12-2 DMF
 CON 16 hours, 80 deg C

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STAGE(2)

RGT F 7647-14-5 NaCl
SOL 67-68-5 DMSO
CON 48 hours, 140 deg C

STAGE(3)

RCT W 616-75-1
RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4
SOL 7732-18-5 Water

STAGE(4)

RCT B 70-11-1
RGT I 127-09-3 AcONa, J 64-19-7 AcOH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) 24 hours, room temperature

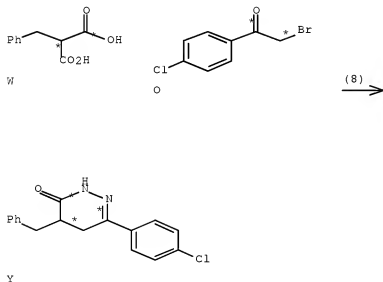
STAGE(5)

RGT K 302-01-2 N2H4
SOL 7732-18-5 Water, 68-12-2 DMF
CON 17 hours, room temperature

PRO X 202800-65-5

NTE solid-supported reagent, Merrifield resin used

RX(8) OF 9 W + O ==> Y



RX(8)

STAGE(1)

RGT D 100-44-7D PhCH2Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)
SOL 68-12-2 DMF

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CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl

SOL 67-68-5 DMSO

CON 48 hours, 140 deg C

STAGE(3)

RCT W 616-75-1

RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4

SOL 7732-18-5 Water

STAGE(4)

RCT O 536-38-9

RGT I 127-09-3 AcONa, J 64-19-7 AcOH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 1 hour, room temperature

SUBSTAGE(2) 24 hours, room temperature

STAGE(5)

RGT K 302-01-2 N2H4

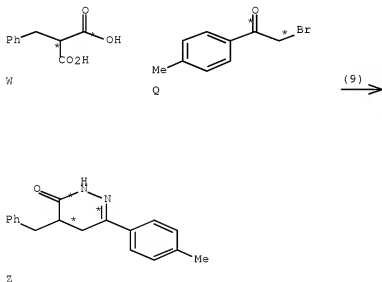
SOL 7732-18-5 Water, 68-12-2 DMF

CON 17 hours, room temperature

PRO Y 202900-75-7

NTE solid-supported reagent, Merrifield resin used

RX(9) OF 9 W + Q ==> Z



RX(9)

STAGE(1)

RGT D 100-44-7D PhCH2Cl, E 19232-39-4 Butanoic acid, 3-oxo-, ethyl ester, ion(1-), sodium (1:1)

SOL 68-12-2 DMF

CON 16 hours, 80 deg C

STAGE(2)

RGT F 7647-14-5 NaCl
 SOL 67-68-5 DMSO
 CON 48 hours, 140 deg C

STAGE(3)

RCT W 616-75-1
 RGT G 108-24-7 Ac2O, H 7664-93-9 H2SO4
 SOL 7732-18-5 Water

STAGE(4)

RCT Q 619-41-0
 RGT I 127-09-3 AcONa, J 64-19-7 AcOH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 1 hour, room temperature
 SUBSTAGE(2) 24 hours, room temperature

STAGE(5)

RGT K 302-01-2 N2H4
 SOL 7732-18-5 Water, 68-12-2 DMF
 CON 17 hours, room temperature

PRO Z 746663-01-4

NTE solid-supported reagent, Merrifield resin used

L91 ANSWER 11 OF 30 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 140:367760 CASREACT [Full-text](#)

TITLE: A New Route for Preparing Coordination Polymers from Hydrothermal Reactions Involving in Situ Ligand Synthesis

AUTHOR(S): Hu, Xi-Xue; Xu, Ji-Qing; Cheng, Peng; Chen, Xiao-Yan; Cui, Xiao-Bing; Song, Jiang-Feng; Yang, Guang-Di; Wang, Tie-Gang

CORPORATE SOURCE: College of Chemistry and State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, Changchun, 130023, Peop. Rep. China

SOURCE: Inorganic Chemistry (2004), 43(7), 2261-2266
 CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

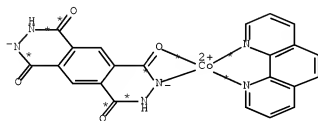
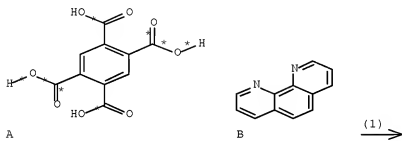
AB The coordination chemical of an inorg. cobalt salt and the organic ligands H4bbh (benzene-1,2,4,5-bihydrazide) and H3bcbh (benzene-4-carboxylate-1,2-bihydrazide) generated through the in situ hydrothermal acylate reaction of H4bta (benzene-1,2,4,5-tetracarboxylic acid) and H3btc (benzene-1,2,4-tricarboxylic acid) with hydrazine hydrate, resp., was studied. Three new coordination polymers were prepared and fully characterized by IR spectroscopy, elemental anal., and single-crystal x-ray diffraction. [Co(μ_3 -H2bbh)(phen)]_n (1, triclinic space group P₂12₁1 with a 9.762(4), b 10.169(4), c 11.143(4) Å, α 80.96(3), β 64.49(3), γ 71.88(3)°, Z = 2) was synthesized from the reaction of CoCl₂·6H₂O, H4bta (benzene-1,2,4,5-tetracarboxylic acid), N2H4·H2O, phen (1,10-phenanthroline) and H2O, and consists of 1-dimensional double-chains. [Co(μ_4 -H2bbh)(H2O)2]_n (2, monoclinic space group P2(1)/c with a 6.8687(5), b 7.5943(6), c 10.0401(6) Å, β 95.250(4)°, Z = 2) was generated by the combination of CoCl₂·6H₂O, H4bta, N2H4·H2O, and H2O. It adopts a three-dimensional structural motif in the

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solid state with channels consisting of 20-numbered rings. $[\text{Co}(\mu_3\text{-Hbcbh})(\text{bpy})]_n$ (3, monoclinic space group Cc with a 9.9464(13), b 23.685(5), c 7.9491(16) Å, β 117.677(13)°, Z = 4) was obtained from the mixture of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$, H3btc (benzene-1,2,4-tricarboxylic acid), bpy (2,2'-bipyridyl), and H_2O , and features a two-dimensional plane. The results of magnetic research indicate that there exist antiferromagnetic interactions between Co centers in both compds. 1 and 2.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 3 A + B ==> C

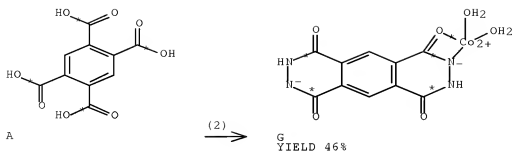


C
YIELD 41%

RX(1) RCT A 89-05-4, B 66-71-7
RGT D 7803-57-8 N2H4-H2O, E 7646-79-3 CoCl2
PRO C 681439-74-7
SOL 7732-18-5 Water
CON SUBSTAGE(1) 4 days, 170 deg C
SUBSTAGE(2) 170 deg C -> room temperature

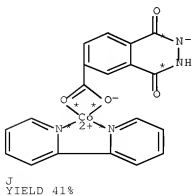
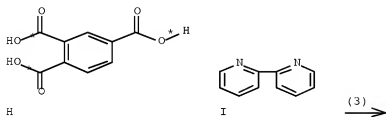
RX(2) OF 3 A ==> G

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RX(2) RCT A 89-05-4
 RGT D 7803-57-9 N2H4-H2O, E 7646-79-9 CoCl2, B
 66-71-7 1,10-Phenanthroline
 PRO G 681439-75-8
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 4 days, 170 deg C
 SUBSTAGE(2) 170 deg C -> room temperature

RX(3) OF 3 H + I ==> J



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RX(3) RCT H 523-44-9, I 366-18-7
 RGT D 7863-57-8 N2H4-H2O, E 7646-79-9 CoCl2
 PRO J 681439-76-9
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 4 days, 170 deg C
 SUBSTAGE(2) 170 deg C -> room temperature

L91 ANSWER 12 OF 30 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 139:292230 CASREACT Full-text

TITLE: Synthesis and SAR of Thrombin Inhibitors Incorporating a Novel 4-Amino-Morpholinone Scaffold: Analysis of X-ray Crystal Structure of Enzyme Inhibitor Complex

AUTHOR(S): Nilsson, Jonas W.; Kvarnstrom, Ingemar; Musil, Djordje; Nilsson, Ingemar; Samulesson, Bertil

CORPORATE SOURCE: Department of Chemistry, Linköping University, Linköping, S-581 83, Swed.

SOURCE: Journal of Medicinal Chemistry (2003), 46(19), 3985-4001

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

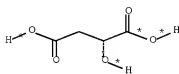
LANGUAGE: English

AB A 4-amino-2-carboxymethyl-3-morpholinone structural motif derived from malic acid has been used to mimic D-Phe-Pro in the thrombin inhibiting tripeptide D-Phe-Pro-Arg. The arginine in D-Phe-Pro-Arg was replaced by the more rigid P1 truncated p-amidinobenzylamine (Pab). These new thrombin inhibitors were used to probe the inhibitor binding site of α -thrombin. The best candidate in this series of thrombin inhibitors exhibits an in vitro IC50 of 0.130 μ M. Interestingly, the stereochem. of the 4-amino-2-carboxymethyl-3-morpholinone motif is reversed for the most active compds. compared to that of a previously reported 2-carboxymethyl-3-morpholinone series. The X-ray crystal structure of the lead inhibitor cocrystd. with α -thrombin is discussed.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(349) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10)

RX(349) ET + 2 B + E + O ==> AH



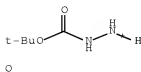
ET



2 B

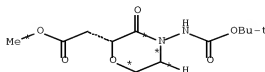


E



O

4
STEPS
→



AH
YIELD 11%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

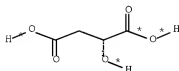
PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9
PRO AH 609846-38-0
SOL 108-88-3 PhMe
CON 3 days, reflux

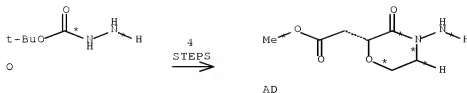
RX(350) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97)
RX(350) ET + 2 B + E + O ==> AD



ET

H3C-CH2-OH
2 B

Br-CH2-CH=CH2
E



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

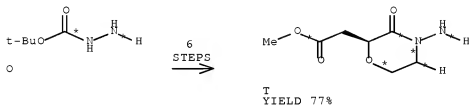
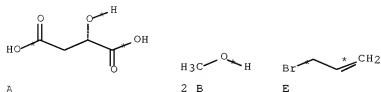
RX(96) RCT O 879-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

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RX(379) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)
 RX(379) A + 2 B + E + O ==> T



RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

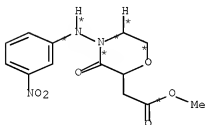
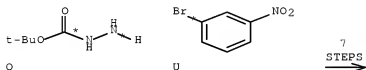
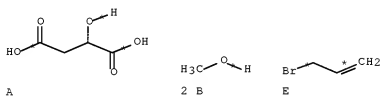
RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

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RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(426) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7)
 RX(426) A + 2 B + E + O + U ==> V



V
 YIELD 33%

RX(1) RCT A 57-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2

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```
PRO C 617-55-0
CON room temperature

RX(2)  RCT C 617-55-0, E 106-95-6
      RGT G 20667-12-3 Ag2O
      PRO F 297749-53-2
      SOL 108-88-3 PhMe
      CON room temperature
      NTE other product also detected

RX(3)  RCT F 297749-53-2

      STAGE(1)
      RGT J 7529-22-8 Me-morpholineoxide
      CAT 20816-12-0 OsO4
      SOL 7732-18-5 Water, 109-99-9 THF
      CON room temperature

      STAGE(2)
      RGT K 7790-23-5 NaIO4
      SOL 7732-18-5 Water, 109-99-9 THF
      CON room temperature

PRO I 441764-54-1

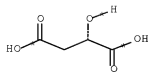
RX(4)  RCT I 441764-54-1, O 870-46-2
      PRO P 609846-32-4
      SOL 108-88-3 PhMe
      CON SUBSTAGE(1) room temperature -> 65 deg C
      SUBSTAGE(2) overnight, 65 deg C

RX(5)  RCT P 609846-32-4
      RGT R 1333-74-0 H2
      PRO Q 609846-33-5
      CAT 7440-05-3 Pd
      SOL 109-99-9 THF
      CON 18 hours, room temperature

RX(6)  RCT Q 609846-33-5
      PRO T 609846-34-6
      SOL 7732-18-5 Water
      CON 7 hours, 60 deg C
      NTE key intermediate

RX(7)  RCT T 609846-34-6, U 585-79-5
      RGT W 534-17-8 Cs2CO3
      PRO V 609846-35-7
      CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-
      diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
      SOL 108-88-3 PhMe
      CON SUBSTAGE(1) room temperature
      SUBSTAGE(2) room temperature -> 95 deg C
      SUBSTAGE(3) 19 hours, 95 deg C

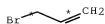
RX(427) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8)
RX(427) 2 A + 4 B + 2 E + 2 O + 3 Z ==>
AA + AB
```



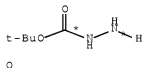
2 A



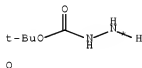
4 B



2 E



O

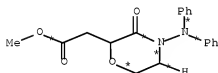
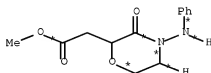


O



3 Z

7
STEPS
→

AA
YIELD 58%AB
YIELD 58%

- RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature
- RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected
- RX(3) RCT F 297749-53-2

STAGE(1)

- RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

- RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

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PRO I 441764-54-1

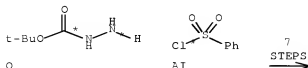
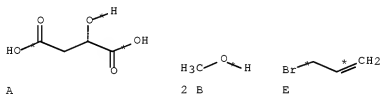
RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

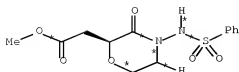
RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1
 RGT W 534-17-8 Cs2CO3
 PRO AA 609846-36-8, AB 609847-53-2
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 95 deg C
 SUBSTAGE(3) 19 hours, 95 deg C

RX(428) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(12)
 RX(428) A + 2 B + E + O + AI ==> AK



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AK
YIELD 85%

```

RX(1)      RCT  A 97-67-6, B 67-56-1
            RGT  D 7719-09-7 SOCl2
            PRO  C 617-55-0
            CON  room temperature

RX(2)      RCT  C 617-55-0, E 106-95-6
            RGT  G 20667-12-3 Ag2O
            PRO  F 297749-53-2
            SOL  108-88-3 PhMe
            CON  room temperature
            NTE  other product also detected

RX(3)      RCT  F 297749-53-2

            STAGE(1)
            RGT  J 7529-22-8 Me-morpholineoxide
            CAT  20816-12-0 OsO4
            SOL  7732-18-5 Water, 109-99-9 THF
            CON  room temperature

            STAGE(2)
            RGT  K 7790-28-5 NaIO4
            SOL  7732-18-5 Water, 109-99-9 THF
            CON  room temperature

PRO  I 441764-54-1

RX(4)      RCT  I 441764-54-1, O 870-46-2
            PRO  P 609846-32-4
            SOL  108-88-3 PhMe
            CON  SUBSTAGE(1) room temperature -> 65 deg C
                SUBSTAGE(2) overnight, 65 deg C

RX(5)      RCT  P 609846-32-4
            RGT  R 1333-74-0 H2
            PRO  Q 609846-33-5
            CAT  7440-05-3 Pd
            SOL  109-99-9 THF
            CON  18 hours, room temperature

RX(6)      RCT  Q 609846-33-5
            PRO  T 609846-34-6
            SOL  7732-18-5 Water
            CON  7 hours, 60 deg C
            NTE  key intermediate

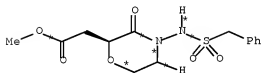
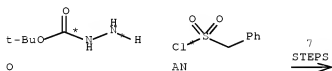
RX(12)     RCT  T 609846-34-6, AI 98-09-9
  
```

PRO AK 609846-40-4
SOL 110-86-1 Pyridine
CON 20 hours, room temperature

$\text{HO}-\text{C}(=\text{O})-\text{CH}_2-\text{CH}(\text{O}-\text{H})-\text{C}(=\text{O})-\text{OH}$
 A

$\text{H}_3\text{C}-\text{O}-\text{H}$
 2 B

$\text{Br}^- - \text{CH}_2 - \text{CH}=\text{CH}_2$
 E



RX(1)	RCT	A 97-67-6, B 67-56-1
	RGT	D 7719-09-7 SOC12
	PRO	C 617-55-0
	CON	room temperature
RX(2)	RCT	C 617-55-0, E 106-95-6
	RGT	G 20667-12-3 Ag2O
	PRO	F 297749-53-2
	SOL	108-88-3 PhMe
	CON	room temperature
	NTE	other product also detected
RX(3)	RCT	F 297749-53-2

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SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

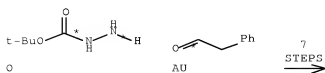
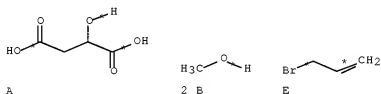
RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

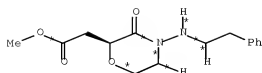
RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(15) RCT T 609846-34-6, AN 1939-99-7
PRO AP 609846-43-7
SOL 110-86-1 Pyridine
CON SUBSTAGE(1) 24 hours, room temperature
SUBSTAGE(2) room temperature -> 35 deg C
SUBSTAGE(3) 3 days, 35 deg C

RX(430) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(19)
RX(430) A + 2 B + E + O + AU ==> AW





AW
YIELD 63%

RX(1) RCT A 27-67-6, B 67-56-1
RGT D 7719-09-7 SOCl₂
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag₂O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 370-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H₂
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C

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NTE key intermediate

RX(19) RCT T 609846-34-6, AU 122-78-1

STAGE(1)

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

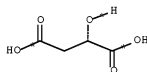
SOL 109-99-9 THF

CON 2 hours, room temperature

PRO AW 609846-47-1

RX(431) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(21)

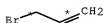
RX(431) A + 2 B + E + O + AX ==> BA



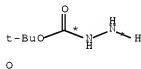
A



2 B



E

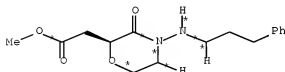


O



AX

7
STEPS
→



BA

YIELD 85%

RX(1) RCT A 97-67-6, B 67-56-1

RGT D 7719-09-7 SOC12

PRO C 617-55-0

CON room temperature

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RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(21) RCT T 609846-34-6, AX 104-53-0

STAGE(1)

SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 5 hours, 70 deg C

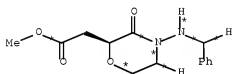
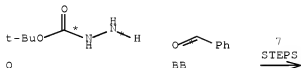
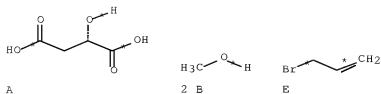
STAGE(2)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 3 hours, room temperature

PRO BA 609846-50-6

RX(432) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(23)
RX(432) A + 2 B + E + O + BB ==> EE

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BE
YIELD 56%

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

 RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

 RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 370-45-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(23) RCT T 609846-34-6, BB 100-52-7

STAGE(1)

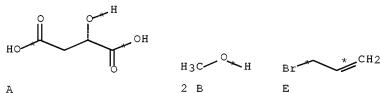
RGT BD 1125-88-8 PhCH(OMe)2
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 80 deg C
 SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)

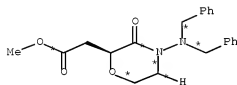
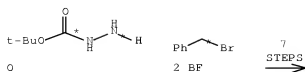
RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 5 minutes, room temperature

PRO BE 609846-52-8

RX(433) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(24)
 RX(433) A + 2 B + E + O + 2 BF ==> BG



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BG
 YIELD 60%

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5

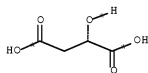
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CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(24) RCT T 609846-34-6, BF 100-39-0
RGT BH 7087-68-5 EtN(Pr-i)2, BI 144-55-8 NaHCO3
PRO BG 609846-53-9
CAT 10377-51-3 LiI
SOL 68-12-2 DMF
CON SUBSTAGE(1) room temperature -> 50 deg C
SUBSTAGE(2) 7 hours, 50 deg C

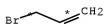
RX(434) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(25)
RX(434) A + 2 B + E + O + BL ==> BM



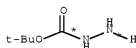
A



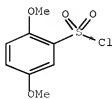
2 B



E

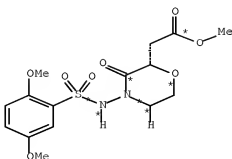


O



BL

7
STEPS
→



BM
YIELD 82%

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOC12
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

 STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

 STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

 PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

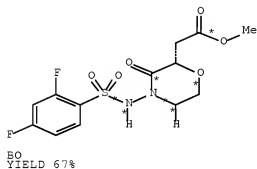
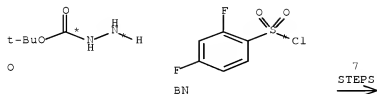
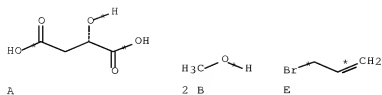
RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(25) RCT T 609846-34-6, BL 1483-28-9
 PRO BM 609846-54-0
 SOL 110-86-1 Pyridine
 CON 24 hours, room temperature

RX(435) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(26)
 RX(435) A + 2 B + E + O + BN ==> BG

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RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

 STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2

PRO P 609846-32-4

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4

RGT R 1333-74-0 H2

PRO Q 609846-33-5

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5

PRO T 609846-34-6

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

NTE key intermediate

RX(26) RCT T 609846-34-6, BN 13918-92-8

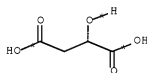
PRO BO 609846-55-1

SOL 110-86-1 Pyridine

CON 24 hours, room temperature

RX(436) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(27)

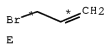
RX(436) A + 2 B + E + O + BP ==> BQ



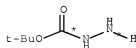
A



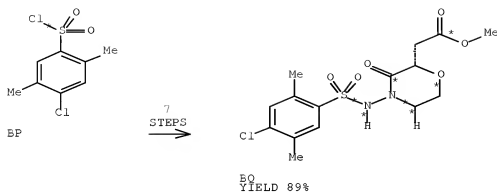
2 B



E



O



RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl₂
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag₂O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7750-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H₂
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

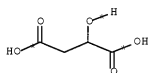
RX(6) RCT Q 609846-33-5
PRO T 609846-34-6

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SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(27) RCT T 609846-34-6, BP 88-49-3
PRO BQ 609846-56-2
SOL 110-86-1 Pyridine
CON 24 hours, room temperature

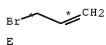
RX(437) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(28)
RX(437) A + 2 B + E + O + BR ==> BS



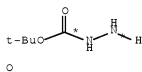
A



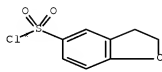
2 B



E

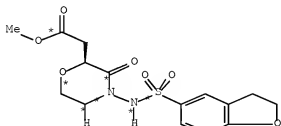


O



BR

7
STEPS
→



BS
YIELD 98%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

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RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

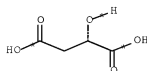
RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(28) RCT T 609846-34-6, BR 115010-11-2
 PRO BS 609846-57-3
 SOL 110-86-1 Pyridine
 CON 90 minutes, room temperature

RX(438) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(29)
 RX(438) A + 2 B + E + C + BT ==> EU



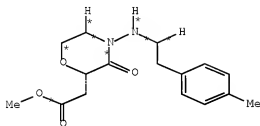
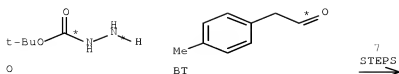
A



2 B



E



BU
YIELD 47%

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl₂
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag₂O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO₄
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-26-5 NaIO₄
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C

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SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(29) RCT T 609846-34-6, BT 104-09-6

STAGE(1)

SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) overnight, 75 deg C

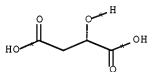
STAGE(2)

RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 24 hours, room temperature

PRO BU 609846-58-4

RX(439) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(75)

RX(439) A + 2 B + E + O + AI + CL + DM ==>
 DU



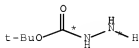
A



2 B



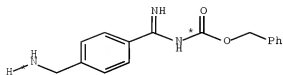
E



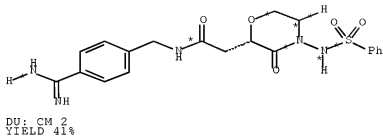
O



AI



● 2 HCl

7
STEPS
→

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 879-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe

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CON  SUBSTAGE(1) room temperature -> 65 deg C
      SUBSTAGE(2) overnight, 65 deg C

RX(5)  RCT  P 609846-32-4
      RGT  R 1333-74-0 H2
      PRO  Q 609846-33-5
      CAT  7440-05-3 Pd
      SOL  109-99-9 THF
      CON  18 hours, room temperature

RX(6)  RCT  Q 609846-33-5
      PRO  T 609846-34-6
      SOL  7732-18-5 Water
      CON  7 hours, 60 deg C
      NTE  key intermediate

RX(75) RCT  T 609846-34-6, AI 98-09-9

      STAGE(1)
      SOL  110-86-1 Pyridine
      CON  20 hours, room temperature

      STAGE(2)
      RGT  BW 1310-65-2 LiOH
      SOL  7732-18-5 Water, 67-56-1 MeOH
      CON  room temperature

      STAGE(3)
      RGT  BX 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  room temperature

      STAGE(4)
      RCT  CL 172348-75-3
      RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
      SOL  68-12-2 DMF
      CON  100 minutes, room temperature

      STAGE(5)
      RGT  R 1333-74-0 H2
      CAT  7440-05-3 Pd
      SOL  7732-18-5 Water, 64-17-5 EtOH
      CON  1 hour, room temperature

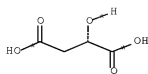
      STAGE(6)
      RCT  DM 64-19-7
      SOL  7732-18-5 Water, 67-56-1 MeOH
      CON  room temperature

PRO  DU 609847-12-3

RX(440) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(78)
RX(440)  A + 2 B + E + O + AN + CL + DM ==>
DX

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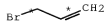
10/595943



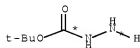
A



2 B



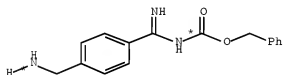
E



O



AN



CL

2 HCl

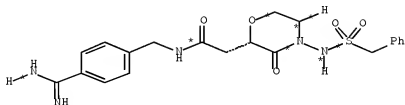


DM

7 STEPS



DX: CM 1
YIELD 8%



DX: CM 2
YIELD 8%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6

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RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(78) RCT T 609846-34-6, AN 1939-99-7

STAGE(1)

SOL 110-86-1 Pyridine
CON SUBSTAGE(1) 24 hours, room temperature
SUBSTAGE(2) room temperature -> 35 deg C
SUBSTAGE(3) 3 days, 35 deg C

STAGE(2)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(4)

RCT CL 172348-75-3

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RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(5)

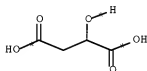
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 1 hour, room temperature

STAGE(6)

RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO DX 609647-18-9

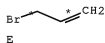
RX(441) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(82)
RX(441) A + 2 B + E + O + AU + CL + DM ==>
EE



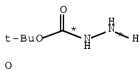
A



2 B



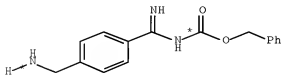
E



O



AU



CL

● 2 HCl

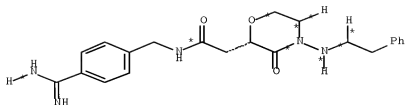


DM

7
STEPS
→



EB: CM 1
YIELD 51%



EB: CM 2
YIELD 51%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7750-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6

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SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(82) RCT T 609846-34-6, AU 122-78-1

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, 60 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 2 hours, room temperature

STAGE(3)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(4)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(5)
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

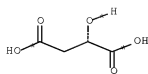
STAGE(6)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 2 hours, room temperature

STAGE(7)
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO EB 609847-26-9

RX(442) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(84)
RX(442) A + 2 B + E + O + AX + CL + DM ==>
ED

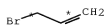
10/595943



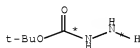
A



B



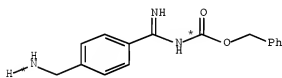
E



O



AX



CL



2

HCl



DM



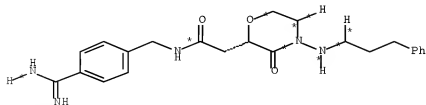
7

STEPS



ED: CM 1

YIELD 15%



ED: CM 2

YIELD 15%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(84) RCT T 609846-34-6, AX 104-53-0

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 5 hours, 70 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 3 hours, room temperature

STAGE(3)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

STAGE(5)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 2 hours, room temperature

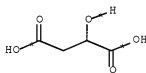
STAGE(7)

RCT DM 64-19-7
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

PRO ED 609847-30-5

RX(443) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(88)

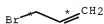
RX(443) A + 2 B + E + O + 2 BF + CL + DM
 ==> EL



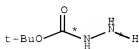
A



2 B



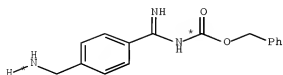
E



O

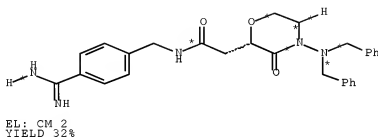


2 BF



CL

● 2 HCl

7
STEPS
→

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4

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```
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
    SUBSTAGE(2) overnight, 65 deg C

RX(5)    RCT P 609846-32-4
        RGT R 1333-74-0 H2
        PRO Q 609846-33-5
        CAT 7440-05-3 Pd
        SOL 109-99-9 THF
        CON 18 hours, room temperature

RX(6)    RCT Q 609846-33-5
        PRO T 609846-34-6
        SOL 7732-18-5 Water
        CON 7 hours, 60 deg C
        NTE key intermediate

RX(88)   RCT T 609846-34-6, BF 100-39-0

        STAGE(1)
        RGT BH 7087-68-5 EtN(Pr-i)2, BI 144-55-8 NaHCO3
        CAT 10377-51-2 LiI
        SOL 68-12-2 DMF
        CON SUBSTAGE(1) room temperature -> 50 deg C
            SUBSTAGE(2) 7 hours, 50 deg C

        STAGE(2)
        RGT BW 1310-65-2 LiOH
        SOL 7732-18-5 Water, 67-56-1 MeOH
        CON room temperature

        STAGE(3)
        RGT BX 7647-01-0 HCl
        SOL 7732-18-5 Water
        CON room temperature

        STAGE(4)
        RCT CL 172348-75-3
        RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
            1-[bis(dimethylamino)methylene]-, 3-oxide,
            hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
        SOL 68-12-2 DMF
        CON 100 minutes, room temperature

        STAGE(5)
        RGT R 1333-74-0 H2
        CAT 7440-05-3 Pd
        SOL 7732-18-5 Water, 64-17-5 EtOH
        CON 24 hours, room temperature

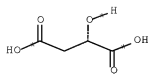
        STAGE(6)
        RCT DM 64-19-7
        SOL 7732-18-5 Water, 67-56-1 MeOH
        CON room temperature

PRO EL 609847-37-2

RX(444) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(89)
RX(444)  A  +  2 B  +  E  +  O  +  BL  +  CL  +  DM  ==>
```

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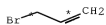
EM



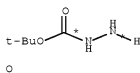
A



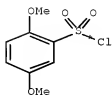
2 B



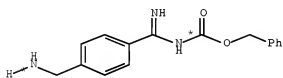
E



O



BL



CL



2

HCl

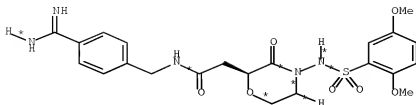


DM

7
STEPS
→



EM: CM 1
YIELD 49%



EM: CM 2
YIELD 49%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

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RX(89) RCT T 609846-34-6, BL 1483-28-9

STAGE(1)

SOL 110-86-1 Pyridine
CON 24 hours, room temperature

STAGE(2)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(4)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 24 minutes, room temperature

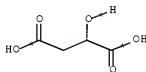
STAGE(6)

RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO EM 609847-39-4

RX(445) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(90)
RX(445) A + 2 B + E + O + BN + CL + DM ==>

EN



A

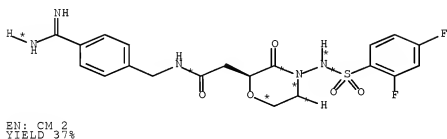
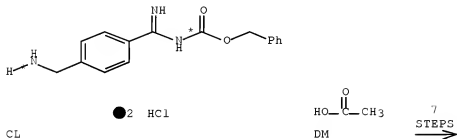
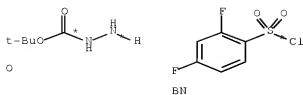


2 B



E

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RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl₂
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag₂O
 PRO F 297749-53-2

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SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7750-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(90) RCT T 609846-34-6, BN 13918-92-8

STAGE(1)
SOL 110-86-1 Pyridine
CON 24 hours, room temperature

STAGE(2)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(3)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(4)
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

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CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 24 minutes, room temperature

STAGE(6)

RCT DM 64-19-7

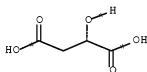
SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

PRO EN 609947-41-8

RX(446) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(91)

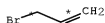
RX(446) 2 A + 4 B + 2 E + 2 O + 2 BP + 2 CL +
2 DM ==> EO + EP



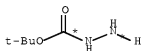
2 A



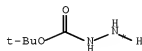
4 B



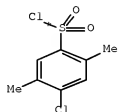
2 E



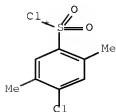
O



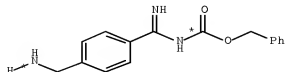
O



BP



BP



2 CL

● 2 HCl



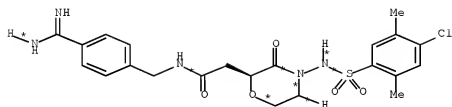
2 DM

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7
STEPS
→



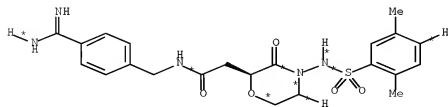
EO: CM 1
YIELD 13%



EO: CM 2
YIELD 13%



EP: CM 1
YIELD 24%



EP: CM 2
YIELD 24%

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RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(91) RCT T 609846-34-6, BP 88-49-3

STAGE(1)
SOL 110-86-1 Pyridine
CON 24 hours, room temperature

STAGE(2)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(3)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water

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CON room temperature

STAGE(4)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 29 minutes, room temperature

STAGE(6)

RCT DM 64-19-7

SOL 7732-18-5 Water, 67-56-1 MeOH

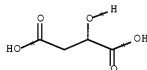
CON room temperature

PRO EO 669847-43-0, EP 609847-45-2

RX(447) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(92)

RX(447) A + 2 B + E + O + BR + CL + DM ==>

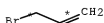
EQ



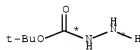
A



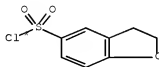
2 B



E

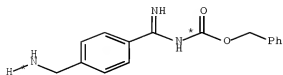


O



BR

10/595943

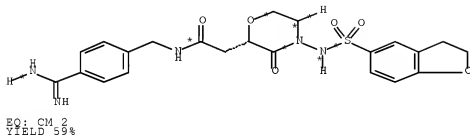


CL

● 2 HCl



7
STEPS
→



RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature


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STAGE(2)
  RGT  K 7790-28-5 NaIO4
  SOL  7732-18-5 Water, 109-99-9 THF
  CON  room temperature

PRO  I 441764-54-1

RX(4)  RCT  I 441764-54-1, O 870-46-2
      PRO  P 609846-32-4
      SOL  108-88-3 PhMe
      CON  SUBSTAGE(1) room temperature -> 65 deg C
          SUBSTAGE(2) overnight, 65 deg C

RX(5)  RCT  P 609846-32-4
      RGT  R 1333-74-0 H2
      PRO  Q 609846-33-5
      CAT  7440-05-3 Pd
      SOL  109-99-9 THF
      CON  18 hours, room temperature

RX(6)  RCT  Q 609846-33-5
      PRO  T 609846-34-6
      SOL  7732-18-5 Water
      CON  7 hours, 60 deg C
      NTE  key intermediate

RX(92) RCT  T 609846-34-6, BR 115010-11-2

STAGE(1)
  SOL  110-86-1 Pyridine
  CON  90 minutes, room temperature

STAGE(2)
  RGT  BW 1310-65-2 LiOH
  SOL  7732-18-5 Water, 67-56-1 MeOH
  CON  room temperature

STAGE(3)
  RGT  BX 7647-01-0 HCl
  SOL  7732-18-5 Water
  CON  room temperature

STAGE(4)
  RCT  CL 172348-75-3
  RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
  SOL  68-12-2 DMF
  CON  100 minutes, room temperature

STAGE(5)
  RGT  R 1333-74-0 H2
  CAT  7440-05-3 Pd
  SOL  7732-18-5 Water, 64-17-5 EtOH, 109-99-9 THF
  CON  1 hour, room temperature

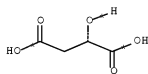
STAGE(6)
  RCT  DM 64-19-7
  SOL  7732-18-5 Water, 67-56-1 MeOH
  CON  room temperature

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10/595943

PRO EQ 665847-47-4

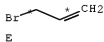
RX(448) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(93)
 RX(448) A + 2 B + E + O + BT + CL + DM ==>
 ER



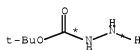
A



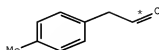
2 B



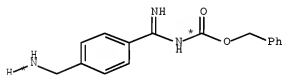
E



O



BT



CL

● 2 HCl



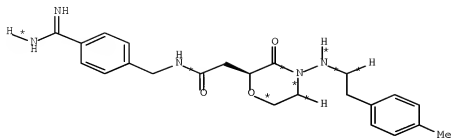
DM

7
STEPS
→



ER: CM 1
YIELD 32%

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ER: CM 2
YIELD 32%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water

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CON 7 hours, 60 deg C
NTE key intermediate

RX(93) RCT T 609846-34-6, BT 104-09-6

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, 75 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 24 hours, room temperature

STAGE(3)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(4)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(5)
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(6)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 25 minutes, room temperature

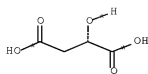
STAGE(7)
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO ER 609847-49-6

RX(503) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7),
RX(30)

RX(503) A + 2 B + E + O + U ==> EV

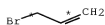
10/595943



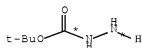
A



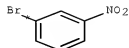
2 B



E

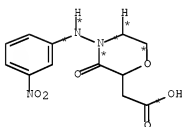


O



U

8
STEPS
→



BV

RX(1) RCT A 57-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(7) RCT T 609846-34-6, U 585-79-5
 RGT W 534-17-8 Cs2CO3
 PRO V 609846-35-7
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 95 deg C
 SUBSTAGE(3) 19 hours, 95 deg C

RX(30) RCT V 609846-35-7

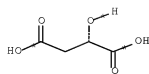
STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO BV 609846-59-5

RX(504) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7),
 RX(44)
 RX(504) A + 2 B + E + O + U + CL ==>
 CN

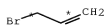
10/595943



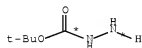
A



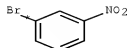
B



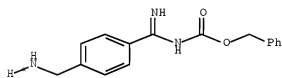
E



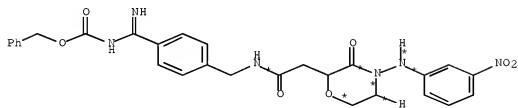
O



U



CL



CM
YIELD 87%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O

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PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(7) RCT T 609846-34-6, U 585-79-5
RGT W 534-17-8 Cs2CO3
PRO V 609846-35-7
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 95 deg C
SUBSTAGE(3) 19 hours, 95 deg C

RX(44) RCT V 609846-35-7

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

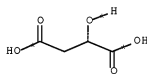
RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

CON 100 minutes, room temperature

PRO CM 669846-74-4

RX(505) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),
RX(46)RX(505) 2 A + 4 B + 2 E + 2 O + 3 Z + CL ==>
CP

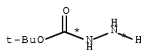
2 A



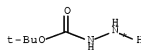
4 B



2 E



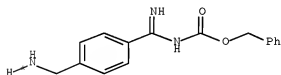
O



O



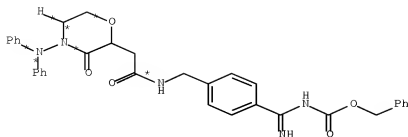
3 Z



● 2 HCl

CL

8
STEPS
→



CP

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RX(1)      RCT  A 37-67-6, B 67-56-1
           RGT  D 7719-09-7 SOC12
           PRO  C 617-55-0
           CON  room temperature

RX(2)      RCT  C 617-55-0, E 106-95-6
           RGT  G 20667-12-3 Ag2O
           PRO  F 297749-53-2
           SOL  108-88-3 PhMe
           CON  room temperature
           NTE  other product also detected

RX(3)      RCT  F 297749-53-2

           STAGE(1)
           RGT  J 7529-22-8 Me-morpholineoxide
           CAT  20816-12-0 OsO4
           SOL  7732-18-5 Water, 109-99-9 THF
           CON  room temperature

           STAGE(2)
           RGT  K 7790-28-5 NaIO4
           SOL  7732-18-5 Water, 109-99-9 THF
           CON  room temperature

PRO  I 441764-54-1

RX(4)      RCT  I 441764-54-1, O 370-46-2
           PRO  P 609846-32-4
           SOL  108-88-3 PhMe
           CON  SUBSTAGE(1) room temperature -> 65 deg C
           SUBSTAGE(2) overnight, 65 deg C

RX(5)      RCT  P 609846-32-4
           RGT  R 1333-74-0 H2
           PRO  Q 609846-33-5
           CAT  7440-05-3 Pd
           SOL  109-99-9 THF
           CON  18 hours, room temperature

RX(6)      RCT  Q 609846-33-5
           PRO  T 609846-34-6
           SOL  7732-18-5 Water
           CON  7 hours, 60 deg C

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NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1
 RGT W 534-17-8 Cs2CO3
 PRO AA 609846-36-8, AB 609847-53-2
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 95 deg C
 SUBSTAGE(3) 19 hours, 95 deg C

RX(46) RCT AA 609846-36-8

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

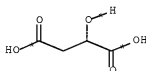
STAGE(3)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene]-, 3-oxide, hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

PRO CP 609846-76-6

RX(506) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8), RX(71)

RX(506) 2 A + 4 B + 2 E + 2 O + 3 Z + CL + DM
 ==> DQ



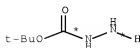
2 A



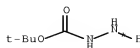
4 B



2 E



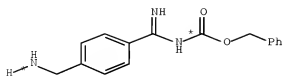
O



O

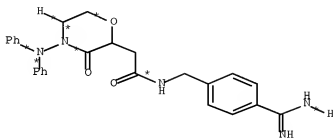


3 Z



CL

● 2 HCl

8
STEPS
➔DQ: CM 1
YIELD 71%DQ: CM 2
YIELD 71%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

RGT K 7739-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1
 RGT W 534-17-8 Cs2CO3
 PRO AA 609846-36-8, AB 609847-53-2
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 95 deg C
 SUBSTAGE(3) 19 hours, 95 deg C

RX(71) RCT AA 609846-36-8

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

STAGE(3)
 RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene]-, 3-oxide, hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-1)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

STAGE(4)
 RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 45 minutes, room temperature

STAGE(5)
 RCT DM 64-19-7
 SOL 7732-18-5 Water, 67-56-1 MeOH

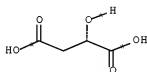
10/595943

CON room temperature

PRO DQ 609847-04-3

RX(507) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),
RX(31)

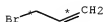
RX(507) 2 A + 4 B + 2 E + 2 O + 3 Z ==>
BY



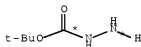
2 A



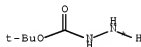
4 B



2 E



O

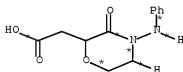


O



3 Z

8
STEPS
→



BY

RX(1) RCT A 57-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1
 RGT W 534-17-8 Cs2CO3
 PRO AA 609846-36-8, AB 609847-53-2
 CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 95 deg C
 SUBSTAGE(3) 19 hours, 95 deg C

RX(31) RCT AB 609847-53-2

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

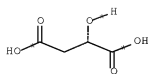
RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO BY 609846-61-9

RX(508) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),
 RX(70)

RX(508) 2 A + 4 B + 2 E + 2 G + 3 Z + CL + DM
 ==> DP

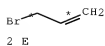
10/595943



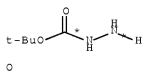
2 A



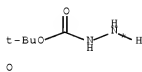
4 B



2 E



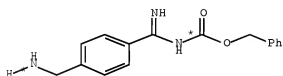
O



O



3 Z



CL

● 2 HCl

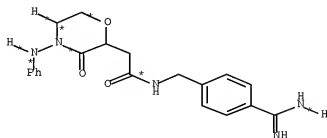


DM

8
STEPS
→



DP: CM 1
YIELD 59%



DP: CM 2
YIELD 59%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0

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CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 370-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1
RGT W 534-17-8 Cs2CO3
PRO AA 609846-36-8, AB 609847-53-2
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 95 deg C
SUBSTAGE(3) 19 hours, 95 deg C

RX(70) RCT AB 609847-53-2

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

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STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(4)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 90 minutes, room temperature

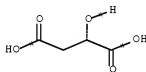
STAGE(5)

RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH

PRO DP 609947-02-1

RX(509) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(12),
RX(35)

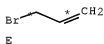
RX(509) A + 2 B + E + O + AI ==> CC



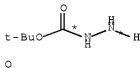
A



2 B



E

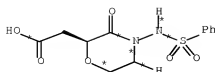


O



AI

8
STEPS
→



CC

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(12) RCT T 609846-34-6, AI 98-09-9
 PRO AK 609846-40-4

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SOL 110-86-1 Pyridine
CON 20 hours, room temperature

RX(35) RCT AK 609846-40-4

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

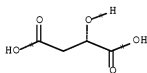
STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

PRO CC 609846-65-3

RX(510) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(15),
RX(53)

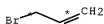
RX(510) A + 2 B + E + O + AN + CL ==>
CW



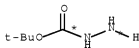
A



2 B



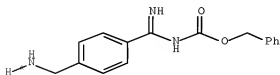
E



O



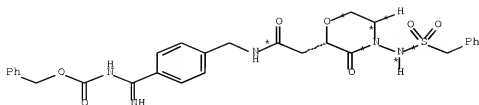
AN



CL

● 2 HCl

8
STEPS
→



CW

RX(1) RCT A 57-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-29-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C

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NTE key intermediate

RX(15) RCT T 609846-34-6, AN 1939-99-7
 PRO AP 609846-43-7
 SOL 110-86-1 Pyridine
 CON SUBSTAGE(1) 24 hours, room temperature
 SUBSTAGE(2) room temperature -> 35 deg C
 SUBSTAGE(3) 3 days, 35 deg C

RX(53) RCT AP 609846-43-7

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

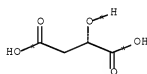
STAGE(3)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

PRO CW 609846-83-5

RX(511) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(19),
 RX(57)

RX(511) A + 2 B + E + O + AU + CL ==>
 DA



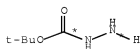
A



2 B



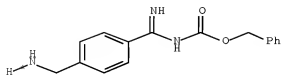
E



O

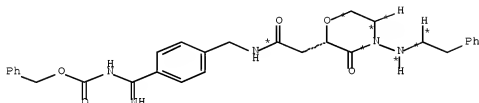


AU



CL

● 2 HCl

⁸
 STEPS


DA

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOC12
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 970-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C

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SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(19) RCT T 609846-34-6, AU 122-78-1

STAGE(1)

SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 2 hours, room temperature

PRO AW 609846-47-1

RX(57) RCT AW 609846-47-1

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

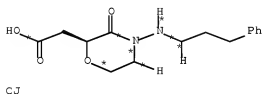
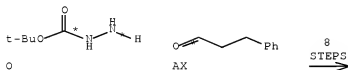
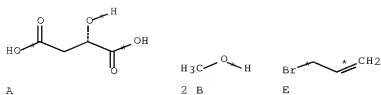
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-1)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

PRO DA 609846-87-9

RX(512) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(21),
RX(42)

RX(512) A + 2 B + E + O + AX ==> CJ

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RX(1) RCT A 57-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-29-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

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RX(4)      RCT  I 441764-54-1, O 870-46-2
           PRO  P 609846-32-4
           SOL  108-88-3 PhMe
           CON  SUBSTAGE(1) room temperature -> 65 deg C
                SUBSTAGE(2) overnight, 65 deg C

RX(5)      RCT  P 609846-32-4
           RGT  R 1333-74-0 H2
           PRO  Q 609846-33-5
           CAT  7440-05-3 Pd
           SOL  109-99-9 THF
           CON  18 hours, room temperature

RX(6)      RCT  Q 609846-33-5
           PRO  T 609846-34-6
           SOL  7732-18-5 Water
           CON  7 hours, 60 deg C
           NTE  key intermediate

RX(21)     RCT  T 609846-34-6, AX 104-53-0

           STAGE(1)
           SOL  108-88-3 PhMe
           CON  SUBSTAGE(1) room temperature
                SUBSTAGE(2) 5 hours, 70 deg C

           STAGE(2)
           RGT  R 1333-74-0 H2
           CAT  7440-05-3 Pd
           SOL  109-99-9 THF
           CON  3 hours, room temperature

           PRO  BA 609846-50-6

RX(42)     RCT  BA 609846-50-6

           STAGE(1)
           RGT  BW 1310-65-2 LiOH
           SOL  7732-18-5 Water, 67-56-1 MeOH
           CON  room temperature

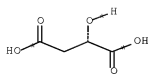
           STAGE(2)
           RGT  BX 7647-01-0 HCl
           SOL  7732-18-5 Water
           CON  room temperature

           PRO  CJ 609846-72-2

RX(513) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(23),
           RX(62)
RX(513)  A  + 2 B  + E  + O  + BB  + CL  ==>
           DF

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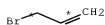
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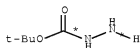
A



2 B



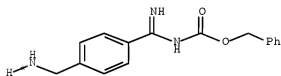
E



O



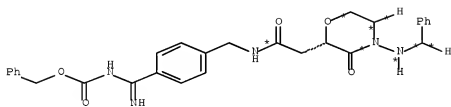
BB



CL

● 2 HCl

8
STEPS
→



DF

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe

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CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(23) RCT T 609846-34-6, BB 100-52-7

STAGE(1)
RGT BD 1125-88-8 PhCH(OMe)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 80 deg C
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 5 minutes, room temperature

PRO BE 609846-52-8

RX(62) RCT BE 609846-52-8

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

10/595943

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

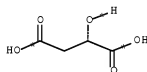
PRO DF 609946-92-6

RX(514) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(23),

RX(87)

RX(514) A + 2 B + E + O + BB + CL + DM ==>

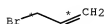
EN



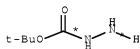
A



2 B



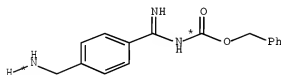
E



O



BB



CL

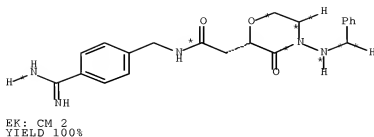
● 2 HCl



DM

8
STEPS
→

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RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

10/595943

RX(23) RCT T 609846-34-6, BB 100-52-7

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)₂
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 80 deg C
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)

RGT R 1333-74-0 H₂
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 5 minutes, room temperature

PRO BE 609846-52-8

RX(87) RCT BE 609846-52-8

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)₂
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(4)

RGT EG 1493-13-6 F₃CSO₂H, EH 100-66-3 PhOMe
SOL 75-09-2 CH₂Cl₂
CON 15 minutes, 0 deg C

STAGE(5)

RGT EI 121-44-8 Et₃N
CON neutralized

STAGE(6)

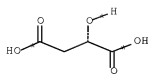
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO EK 609847-35-0

RX(515) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(24),
RX(63)

RX(515) A + 2 B + E + O + 2 BF + CL ==>
D₅

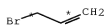
10/595943



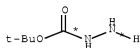
A



2 B



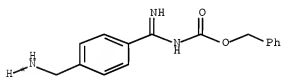
E



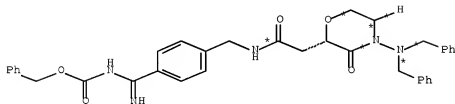
O



2 BF



CL



DG

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2

10/595943

SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

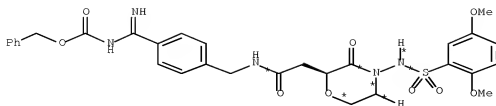
RX(24) RCT T 609846-34-6, BF 100-39-0
RGT BH 7087-68-5 EtN(Pr-i)2, BI 144-55-8 NaHCO3
PRO BG 609846-53-9
CAT 10377-51-2 LiI
SOL 68-12-2 DMF
CON SUBSTAGE(1) room temperature -> 50 deg C
SUBSTAGE(2) 7 hours, 50 deg C

RX(63) RCT BG 609846-53-9

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)
RCT CL 172348-75-3



DH

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl₂
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag₂O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO₄
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO₄
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H₂
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

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RX(25) RCT T 609846-34-6, BL 1483-28-9
 PRO BM 609846-54-0
 SOL 110-86-1 Pyridine
 CON 24 hours, room temperature

RX(64) RCT BM 609846-54-0

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

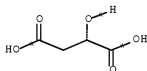
STAGE(3)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

PRO DH 609846-34-8

RX(517) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(26),
 RX(65)

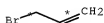
RX(517) A + 2 B + E + O + BN + CL ==>
 DI



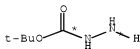
A



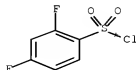
2 B



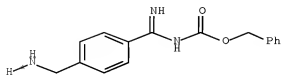
E



O

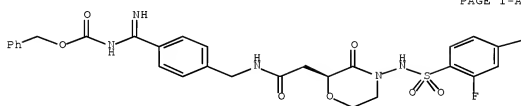


BN



CL
● 2 HCl

8
STEPS
→



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—F
DI

RX(1)	RCT A 97-67-6, B 67-56-1
	RGT D 7719-09-7 SOCl2
	PRO C 617-55-0
	CON room temperature
RX(2)	RCT C 617-55-0, E 106-95-6
	RGT G 20667-12-3 Ag2O
	PRO F 297749-53-2
	SOL 108-88-3 PhMe
	CON room temperature
	NTE other product also detected
RX(3)	RCT F 297749-53-2
STAGE(1)	
	RGT J 7529-22-8 Me-morpholineoxide
	CAT 20816-12-0 OsO4
	SOL 7732-18-5 Water, 109-99-9 THF
	CON room temperature

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      STAGE(2)
      RGT  K 7790-28-5 NaIO4
      SOL  7732-18-5 Water, 109-99-9 THF
      CON  room temperature

PRO  I 441764-54-1

RX(4)  RCT  I 441764-54-1, O 870-46-2
      PRO  P 609846-32-4
      SOL  108-88-3 PhMe
      CON  SUBSTAGE(1) room temperature -> 65 deg C
      SUBSTAGE(2) overnight, 65 deg C

RX(5)  RCT  P 609846-32-4
      RGT  R 1333-74-0 H2
      PRO  Q 609846-33-5
      CAT  7440-05-3 Pd
      SOL  109-99-9 THF
      CON  18 hours, room temperature

RX(6)  RCT  Q 609846-33-5
      PRO  T 609846-34-6
      SOL  7732-18-5 Water
      CON  7 hours, 60 deg C
      NTE  key intermediate

RX(26) RCT  T 609846-34-6, BN 13918-92-8
      PRO  BO 609846-55-1
      SOL  110-86-1 Pyridine
      CON  24 hours, room temperature

RX(65) RCT  BO 609846-55-1

      STAGE(1)
      RGT  BW 1310-65-2 LiOH
      SOL  7732-18-5 Water, 67-56-1 MeOH
      CON  room temperature

      STAGE(2)
      RGT  BX 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  room temperature

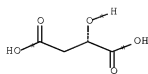
      STAGE(3)
      RCT  CL 172348-75-3
      RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-1)2
      SOL  68-12-2 DMF
      CON  100 minutes, room temperature

PRO  DI 609846-95-5

RX(518) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(27),
      RX(66)
RX(518) A + 2 B + E + O + BP + CL ==>
      DJ

```

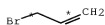
10/595943



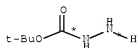
A



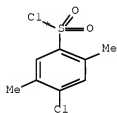
2 B



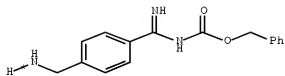
E



O



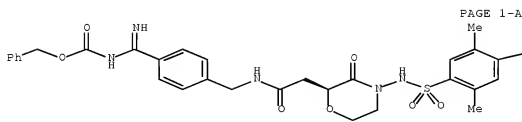
BP



CL

● 2 HCl

8
STEPS
→



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—Cl

DJ

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOCl2
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(27) RCT T 609846-34-6, BP 88-49-3
PRO BQ 609846-56-2
SOL 110-86-1 Pyridine
CON 24 hours, room temperature

RX(66) RCT BQ 609846-56-2

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

10/595943

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

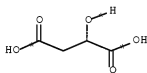
STAGE(3)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

PRO DJ 609846-96-0

RX(519) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(28),
 RX(67)

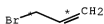
RX(519) A + 2 B + E + O + BR + CL ==>
 DK



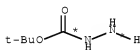
A



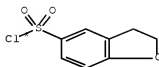
2 B



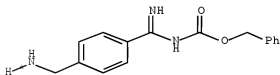
E



O



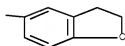
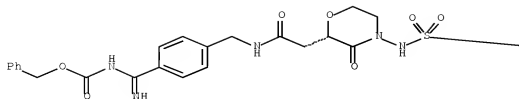
BR



CL

● 2 HCl

8
 STEPS
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DK

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOC12
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

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RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(28) RCT T 609846-34-6, BR 115010-11-2
 PRO BS 609846-57-3
 SOL 110-86-1 Pyridine
 CON 90 minutes, room temperature

RX(67) RCT BS 609846-57-3

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

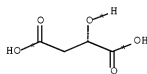
STAGE(3)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

PRO DK 609846-97-1

RX(520) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(29),
 RX(68)

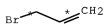
RX(520) A + 2 B + E + O + BT + CL ==>
 DL



A

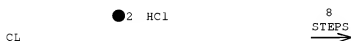
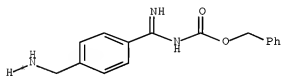
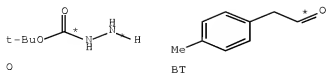


2 B

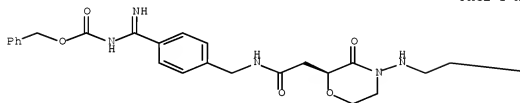


E

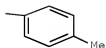
10/595943



PAGE 1-A



PAGE 1-B



DL

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOC12
 PRO C 617-55-0
 CON room temperature

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RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(29) RCT T 609846-34-6, BT 104-09-6

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, 75 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 24 hours, room temperature

PRO BU 609846-58-4

RX(68) RCT BU 609846-58-4

STAGE(1)
RGT BW 1310-65-2 LiOH

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SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

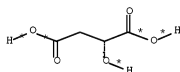
STAGE(3)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

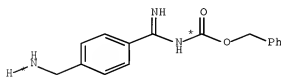
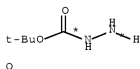
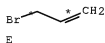
PRO DL 609046-98-2

RX(572) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9), RX(47),
RX(72)

RX(572) ET + 2 B + E + O + AC + CL + DM ==>
DR

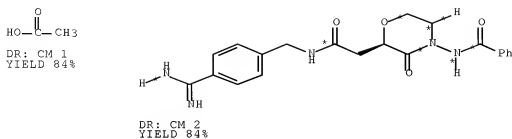


ET



CL





RX(95) RCT EI 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

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NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)

SOL 110-86-1 Pyridine

CON 25 minutes, room temperature

STAGE(2)

SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(47) RCT AE 609846-37-9

STAGE(1)

RGT BW 1310-65-2 LiOH

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature

STAGE(3)

RCT CL 172348-75-3

RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

SOL 68-12-2 DMF

CON 100 minutes, room temperature

PRO CQ 609846-77-7

RX(72) RCT CQ 609846-77-7

STAGE(1)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 7732-18-5 Water, 64-17-5 EtOH

CON 65 minutes, room temperature

STAGE(2)

RCT DM 64-19-7

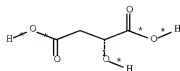
SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

PRO DR 609847-06-5

RX(573) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10), RX(33), RX(48)
RX(573) ET + 2 B + E + O + CL ==> OP

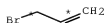
10/595943



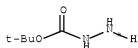
ET



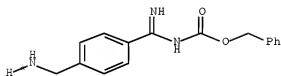
2 B



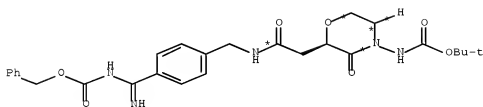
E



O



CL



CR

RX(95) RCT ET 536-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

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SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 879-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9
PRO AH 609846-38-0
SOL 108-88-3 PhMe
CON 3 days, reflux

RX(33) RCT AH 609846-38-0

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

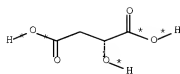
PRO CA 609846-63-1

RX(48) RCT CA 609846-63-1, CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
PRO CR 609846-78-8
SOL 68-12-2 DMF
CON 100 minutes, room temperature

RX(574) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(11), RX(34),
RX(49)
RX(574) ET + 2 B + E + O + AI + CL ==>

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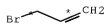
CS



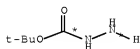
ET



2 B



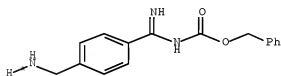
E



O



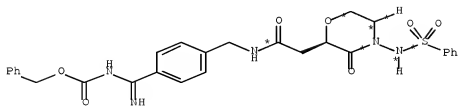
AI



● 2 HCl

CL

7
STEPS
→



CS

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(11) RCT AI 98-09-9, AD 609847-52-1
 PRO AJ 609846-39-1
 SOL 110-86-1 Pyridine
 CON 20 hours, room temperature

RX(34) RCT AJ 609846-39-1

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

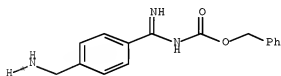
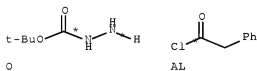
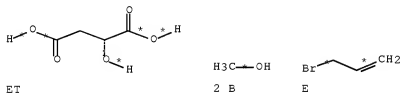
PRO CB 609846-64-2

RX(49) RCT CB 609846-64-2, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,

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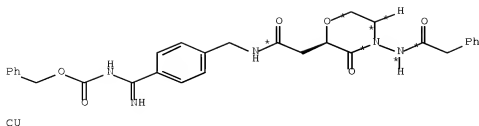
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
PRO CS 605846-79-9
SOL 68-12-2 DMF
CON 100 minutes, room temperature

RX(575) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(13), RX(36),
RX(51)
RX(575) ET + 2 B + E + O + AL + CL ==>
CU



● 2 HCl

7
STEPS
→



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H₂
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(13) RCT AL 103-80-0, AD 609847-52-1
PRO AM 609846-41-5

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SOL 110-86-1 Pyridine
CON 29 hours, room temperature

RX(36) RCT AM 609846-41-5

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

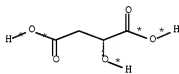
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

PRO CD 609846-66-4

RX(51) RCT CD 609846-66-4, CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
PRO CU 669846-81-3
SOL 68-12-2 DMF
CON 100 minutes, room temperature

RX(576) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(14), RX(37),
RX(52)

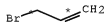
RX(576) ET + 2 B + E + O + AN + CL ==>
CV



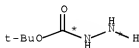
ET



2 B



E

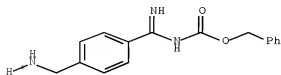


O



AN

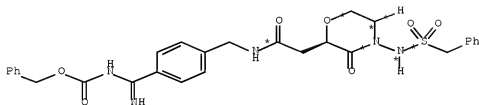
10/595943



CL

● 2 HCl

7
STEPS
→



CV

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

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RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(14) RCT AN 1939-99-7, AD 609847-52-1
 PRO AO 609846-42-6
 SOL 110-86-1 Pyridine
 CON 24 hours, room temperature

RX(37) RCT AO 609846-42-6

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

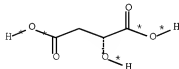
RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CE 609846-67-5

RX(52) RCT CE 609846-67-5, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 PRO CV 609846-82-4
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

RX(577) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16), RX(38),
 RX(54)

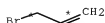
RX(577) ET + 2 B + E + O + AQ + CL ==>
 CX



ET



2 B



E

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)
 SOL 108-88-3 PhMe
 CON 25 hours, room temperature

STAGE(2)
 RGT B 67-56-1 MeOH
 SOL 67-56-1 MeOH
 CON 5 minutes, 40 deg C

PRO AR 609846-44-8

RX(38) RCT AR 609846-44-8

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

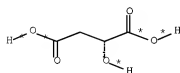
STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CF 609846-68-6

RX(54) RCT CF 609846-68-6, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 PRO CX 609846-84-6
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

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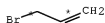
RX(578) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(17), RX(39),
 RX(55)
 RX(578) ET + 2 B + E + O + AS + CL ==>
 CY



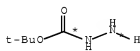
ET



2 B



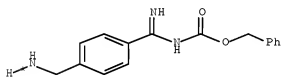
E



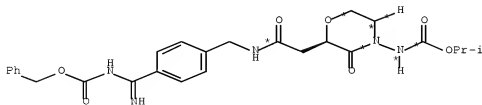
O



AS



CL



CY

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)
 RGT D 7719-09-7 SOC12
 CON room temperature

STAGE(2)
 RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(17) RCT AS 108-23-6, AD 609847-52-1
 PRO AT 609846-45-9
 SOL 108-88-3 PhMe, 110-86-1 Pyridine
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 4 hours

RX(39) RCT AT 609846-45-9

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

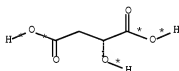
10/595943

PRO CG 609846-69-7

RX(55) RCT CG 609846-69-7, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 PRO CY 609846-85-7
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

RX(579) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(18), RX(40),
 RX(56)

RX(579) ET + 2 B + E + O + AU + CL ==>
 C2



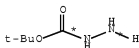
ET



2 B



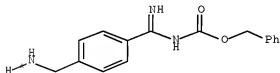
E



O



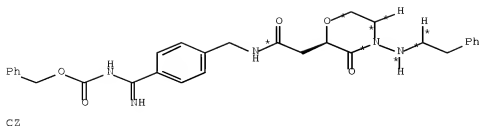
AU



● 2 HCl

CL

7
 STEPS
 →



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(18) RCT AU 122-78-1, AD 609847-52-1

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STAGE(1)
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) overnight, 60 deg C

STAGE(2)
 RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 2 hours, room temperature

PRO AV 609846-46-0

RX(40) RCT AV 609846-46-0

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

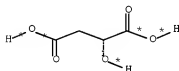
STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CH 609846-70-0

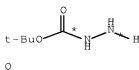
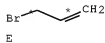
RX(56) RCT CH 609846-70-0, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 PRO CZ 609846-86-8
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

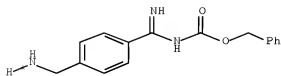
RX(580) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(41),
 RX(58)

RX(580) ET + 2 B + E + O + 3 AX + CL ==>
 DB



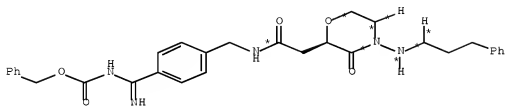
ET





CL

● 2 HCl

⁷
 STEPS
 →


DB

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag₂O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO₄

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-22-5 NaIO₄

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 876-46-2, EU 441764-51-8

PRO ES 609847-51-0

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```
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
    SUBSTAGE(2) overnight, 65 deg C

RX(94)  RCT ES 609847-51-0
        RGT R 1333-74-0 H2
        PRO AG 609847-50-9
        CAT 7440-05-3 Pd
        SOL 109-99-9 THF
        CON 18 hours, room temperature

RX(97)  RCT AG 609847-50-9
        PRO AD 609847-52-1
        SOL 7732-18-5 Water
        CON 7 hours, 60 deg C
        NTE key intermediate

RX(20)  RCT AX 104-53-0, AD 609847-52-1

        STAGE(1)
        SOL 108-88-3 PhMe
        CON SUBSTAGE(1) room temperature
            SUBSTAGE(2) 24 hours, 70 deg C

        STAGE(2)
        RGT R 1333-74-0 H2
        CAT 7440-05-3 Pd
        SOL 109-99-9 THF
        CON 70 minutes, room temperature

        PRO AY 609846-48-2, AZ 609846-49-3

RX(41)  RCT AY 609846-48-2

        STAGE(1)
        RGT BW 1310-65-2 LiOH
        SOL 7732-18-5 Water, 67-56-1 MeOH
        CON room temperature

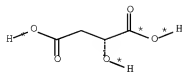
        STAGE(2)
        RGT BX 7647-01-0 HCl
        SOL 7732-18-5 Water
        CON room temperature

        PRO CI 609846-71-1

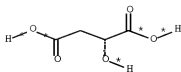
RX(58)  RCT CI 609846-71-1, CL 172348-75-3
        RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
            1-[bis(dimethylamino)methylene]-, 3-oxide,
            hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
        PRO DB 609846-86-3
        SOL 68-12-2 DMF
        CON 100 minutes, room temperature

RX(581) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(60),
RX(85)
RX(581) 2 ET + 2 B + 2 E + 2 O + 3 AX + CL +
DM ==> EE
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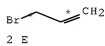
ET



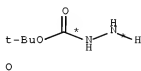
ET



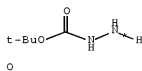
2 B



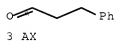
2 E



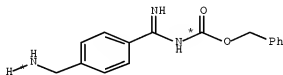
O



O



3 AX



CL

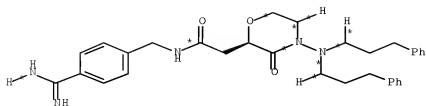


DM

7
STEPS
→



EE: CM $\frac{1}{1}$
YIELD 75%



EE: CM 2
YIELD 75%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

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STAGE(1)
  SOL 108-88-3 PhMe
  CON SUBSTAGE(1) room temperature
      SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)
  RGT R 1333-74-0 H2
  CAT 7440-05-3 Pd
  SOL 109-99-9 THF
  CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(60) RCT AZ 609846-49-3

STAGE(1)
  RGT BW 1310-65-2 LiOH
  SOL 7732-18-5 Water, 67-56-1 MeOH
  CON room temperature

STAGE(2)
  RGT BX 7647-01-0 HCl
  SOL 7732-18-5 Water
  CON room temperature

STAGE(3)
  RCT CL 172348-75-3
  RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
  SOL 68-12-2 DMF
  CON 100 minutes, room temperature

PRO DD 609846-90-4

RX(85) RCT DD 609846-90-4

STAGE(1)
  RGT R 1333-74-0 H2
  CAT 7440-05-3 Pd
  SOL 7732-18-5 Water, 64-17-5 EtOH, 109-99-9 THF
  CON 3 hours, room temperature

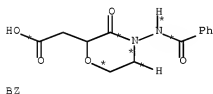
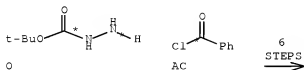
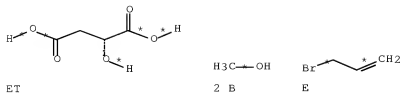
STAGE(2)
  RCT DM 64-19-7
  SOL 7732-18-5 Water, 67-56-1 MeOH
  CON room temperature

PRO EE 609847-32-7

RX(582) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9), RX(32)
RX(582) ET + 2 B + E + O + AC >>> BZ

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

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PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)
 SOL 110-86-1 Pyridine
 CON 25 minutes, room temperature

STAGE(2)
 SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(32) RCT AE 609846-37-9

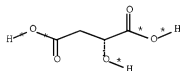
STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO BZ 609846-62-0

RX(583) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9), RX(47)

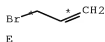
RX(583) ET + 2 B + E + O + AC + CL ==>
 CQ



ET

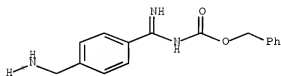
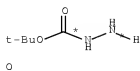


2 B



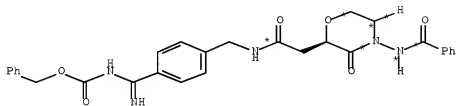
E

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CL
● 2 HCl

6
STEPS
→



CQ
YIELD 50%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature


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      STAGE(4)
      RGT K 7732-18-5 NaIO4
      SOL 7732-18-5 Water, 109-99-9 THF
      CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
      PRO ES 609847-51-0
      SOL 108-88-3 PhMe
      CON SUBSTAGE(1) room temperature -> 65 deg C
      SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
      RGT R 1333-74-0 H2
      PRO AG 609847-50-9
      CAT 7440-05-3 Pd
      SOL 109-99-9 THF
      CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
      PRO AD 609847-52-1
      SOL 7732-18-5 Water
      CON 7 hours, 60 deg C
      NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

      STAGE(1)
      SOL 110-86-1 Pyridine
      CON 25 minutes, room temperature

      STAGE(2)
      SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(47) RCT AE 609846-37-9

      STAGE(1)
      RGT BW 1310-65-2 LiOH
      SOL 7732-18-5 Water, 67-56-1 MeOH
      CON room temperature

      STAGE(2)
      RGT BX 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON room temperature

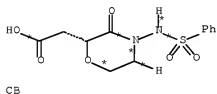
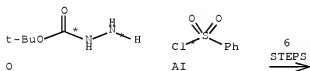
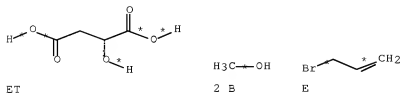
      STAGE(3)
      RCT CL 172348-75-3
      RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
      SOL 68-12-2 DMF
      CON 100 minutes, room temperature

PRO CQ 609846-77-7

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RX(584) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(11), RX(34)
 RX(584) ET + 2 B + E + C + AI ==> CB



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
 CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7759-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

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PRO EU 441764-51-8

RX(96) RCT O 670-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(11) RCT AI 98-09-9, AD 609847-52-1
 PRO AJ 609846-39-1
 SOL 110-86-1 Pyridine
 CON 20 hours, room temperature

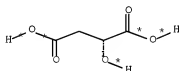
RX(34) RCT AJ 609846-39-1

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CB 609846-64-2

RX(585) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(13), RX(36)
 RX(585) ET + 2 B + E + O + AL ==> CD

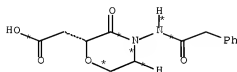
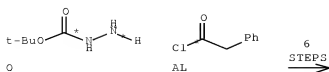


ET

H3C-OH
 2 B

Br-CH2-CH=CH2
 E

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CD

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-29-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(13) RCT AL 103-80-0, AD 609847-52-1
 PRO AM 609846-41-5
 SOL 110-86-1 Pyridine
 CON 29 hours, room temperature

RX(36) RCT AM 609846-41-5

STAGE(1)

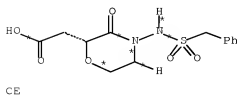
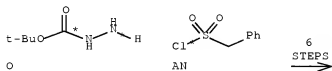
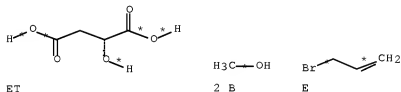
RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CD 609846-66-4

RX(586) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(14), RX(37)
 RX(586) ET + 2 B + E + O + AN ==> CE



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)
 RGT D 7719-09-7 SOC12
 CON room temperature

STAGE(2)
 RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(14) RCT AN 1939-99-7, AD 609847-52-1
 PRO AO 609846-42-6
 SOL 110-86-1 Pyridine
 CON 24 hours, room temperature

RX(37) RCT AO 609846-42-6

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

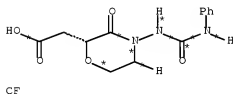
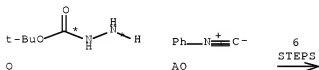
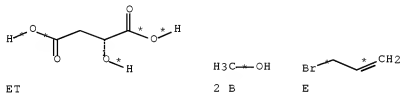
STAGE(2)

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RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

PRO CE 609846-67-5

RX(587) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16), RX(38)
RX(587) ET + 2 B + E + O + AQ ==> CF



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE (1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE (2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE (3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7732-18-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 878-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe

CON 25 hours, room temperature

STAGE(2)

RGT B 67-56-1 MeOH

SOL 67-56-1 MeOH

CON 5 minutes, 40 deg C

PRO AR 609846-44-8

RX(38) RCT AR 609846-44-8

STAGE(1)

RGT BW 1310-65-2 LiOH

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl

SOL 7732-18-5 Water

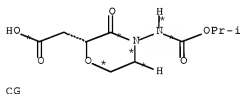
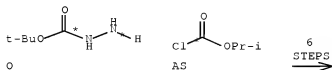
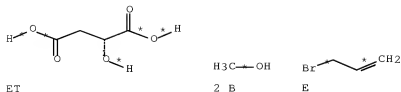
CON room temperature

PRO CF 609846-68-6

RX(588) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(17), RX(39)

RX(588) ET + 2 B + E + O + AS ==> CG

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

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PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(17) RCT AS 108-23-6, AD 609847-52-1
 PRO AT 609846-45-9
 SOL 108-88-3 PhMe, 110-86-1 Pyridine
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 4 hours

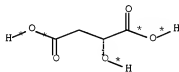
RX(39) RCT AT 609846-45-9

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CG 609846-69-7

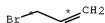
RX(589) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(18), RX(40)
 RX(589) ET + 2 B + E + O + AU ==> CH



ET

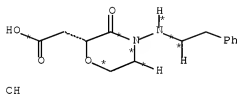
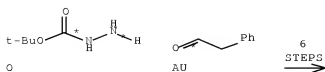


2 B



E

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-29-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(18) RCT AU 122-78-1, AD 609847-52-1

STAGE(1)
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) overnight, 60 deg C

STAGE(2)
 RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 2 hours, room temperature

PRO AV 609846-46-0

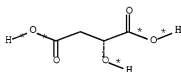
RX(40) RCT AV 609846-46-0

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

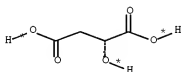
STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CH 609846-70-0

RX(590) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(41)
 RX(590) 2 ET + 2 B + 2 E + 2 C + 3 AX ==>
 C1



ET



ET

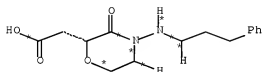
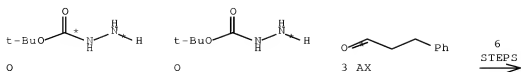
H3C-OH

2 B



2 E

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-29-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94)

RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)
 RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

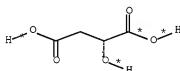
RX(41) RCT AY 609846-48-2

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

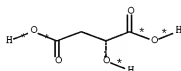
STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CI 609846-71-1

RX(591) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(43)
 RX(591) 2 ET + 2 B + 2 E + 2 O + 3 AX ==>
 CK



ET



ET

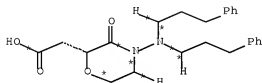
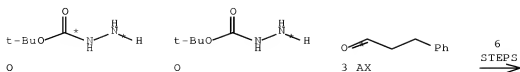
H3C-OH

2 B



2 E

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CK

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

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RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)
 RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

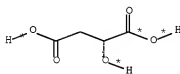
RX(43) RCT AZ 609846-49-3

STAGE(1)
 RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

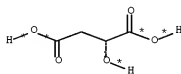
STAGE(2)
 RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CK 609846-73-3

RX(592) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20), RX(60)
 RX(592) 2 ET + 2 B + 2 E + 2 O + 3 AX + CL
 ==> DD



ET



ET



2 B



2 E


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      STAGE(4)
      RGT K 7790-28-5 NaIO4
      SOL 7732-18-5 Water, 109-99-9 THF
      CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
      PRO ES 609847-51-0
      SOL 108-88-3 PhMe
      CON SUBSTAGE(1) room temperature -> 65 deg C
      SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
      RGT R 1333-74-0 H2
      PRO AG 609847-50-9
      CAT 7440-05-3 Pd
      SOL 109-99-9 THF
      CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
      PRO AD 609847-52-1
      SOL 7732-18-5 Water
      CON 7 hours, 60 deg C
      NTE key intermediate

RX(20) RCT AX 104-53-0, AD 609847-52-1

      STAGE(1)
      SOL 108-88-3 PhMe
      CON SUBSTAGE(1) room temperature
      SUBSTAGE(2) 24 hours, 70 deg C

      STAGE(2)
      RGT R 1333-74-0 H2
      CAT 7440-05-3 Pd
      SOL 109-99-9 THF
      CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(60) RCT AZ 609846-49-3

      STAGE(1)
      RGT BW 1310-65-2 LiOH
      SOL 7732-18-5 Water, 67-56-1 MeOH
      CON room temperature

      STAGE(2)
      RGT BX 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON room temperature

      STAGE(3)
      RCT CL 172348-75-3
      RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
      1-[bis(dimethylamino)methylene]-, 3-oxide,
      hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
      SOL 68-12-2 DMF

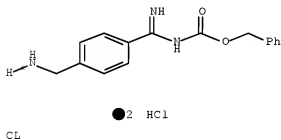
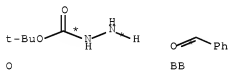
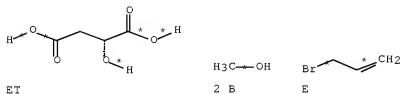
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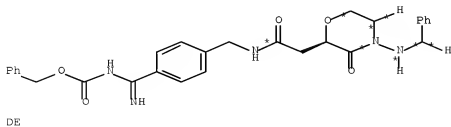
CON 100 minutes, room temperature

PRO DD 609846-90-4

RX(593) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(22), RX(61)
 RX(593) ET + 2 B + E + G + BB + CL ==>
 DE



6
 STEPS
 →



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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-23-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9

PRO AD 609847-52-1

SOL 7732-18-5 Water

CON 7 hours, 60 deg C

NTE key intermediate

RX(22) RCT BB 100-52-7, AD 609847-52-1

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)2

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 80 deg C

SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON 5 minutes, room temperature

PRO BC 609846-51-7

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RX(61) RCT BC 609846-51-7

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

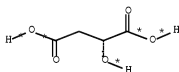
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

PRO DE 609846-91-5

RX(594) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(22), RX(86)

RX(594) ET + 2 B + E + O + BB + CL ==>

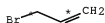
EF



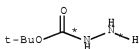
ET



2 B



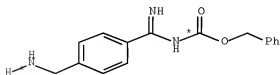
E



O



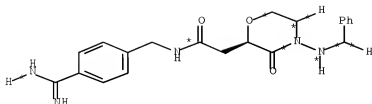
BB



● 2 HCl

CL

6
STEPS
→



EF
YIELD 100%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H₂
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water

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CON 7 hours, 60 deg C
NTE key intermediate

RX(22) RCT BB 100-52-7, AD 609847-52-1

STAGE(1)
RGT BD 1125-88-8 PhCH(OMe)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 80 deg C
SUBSTAGE(2) 2 days, 80 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 5 minutes, room temperature

PRO BC 609846-51-7

RX(86) RCT BC 609846-51-7

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

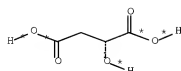
STAGE(4)
RGT EG 1493-13-6 F3CSO2H, EH 100-66-3 PhOMe
SOL 75-09-2 CH2Cl2
CON 15 minutes, 0 deg C

STAGE(5)
RGT EI 121-44-8 Et3N
CON neutralized

PRO EF 609847-33-8

RX(595) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10), RX(33)
RX(595) ET + 2 B + E + O ==> CA

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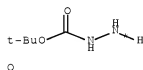
ET



2 B

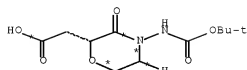


E



O

5
STEPS
→



CA

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6

RGT G 20667-12-3 Ag2O

SOL 108-88-3 PhMe

CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide

CAT 20816-12-0 OsO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

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CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9
 PRO AH 609846-38-0
 SOL 108-88-3 PhMe
 CON 3 days, reflux

RX(33) RCT AH 609846-38-0

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

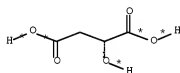
STAGE(2)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

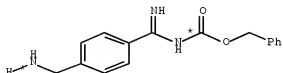
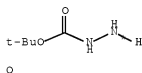
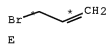
PRO CA 609846-63-1

RX(596) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(10), RX(73)

RX(596) ET + 2 B + E + O + CL + DM ==>
 DS



ET



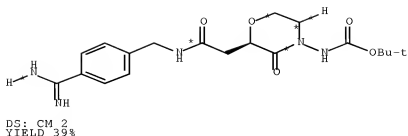
CL

● 2 HCl



5
 STEPS
 ➡

CC(=O)O
 DS: CM 1
 YIELD 39%



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
 CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(10) RCT AG 609847-50-9

PRO AH 609846-38-0
 SOL 108-88-3 PhMe
 CON 3 days, reflux

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RX(73) RCT AH 609846-38-0

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(4)

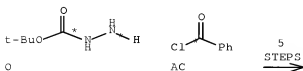
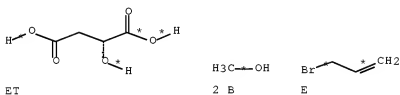
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 45 minutes, room temperature

STAGE(5)

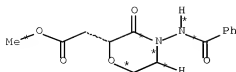
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO DS 609847-06-7

RX(597) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(9)
RX(597) ET + 2 B + E + O + AC ==> AE



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AE
YIELD 97%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(9) RCT AC 98-88-4, AD 609847-52-1

STAGE(1)

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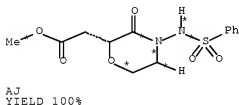
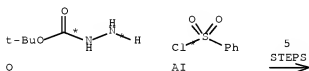
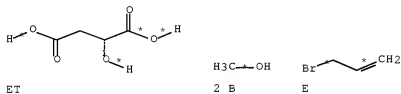
SOL 110-86-1 Pyridine
CON 25 minutes, room temperature

STAGE(2)

SOL 7732-18-5 Water

PRO AE 609846-37-9

RX(598) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(11)
RX(598) ET + 2 B + E + O + AI ==> AJ



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

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RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

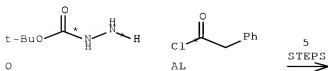
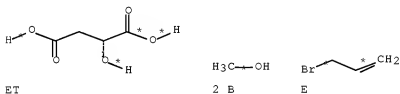
RX(96) RCT O 670-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

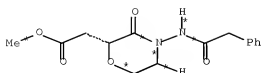
RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(11) RCT AI 98-09-9, AD 609847-52-1
 PRO AJ 609846-39-1
 SOL 110-86-1 Pyridine
 CON 20 hours, room temperature

RX(599) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(13)
 RX(599) ET + 2 B + E + O + AL ==> AM





AM
YIELD 49%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 670-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

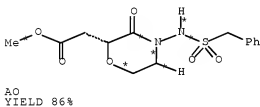
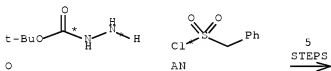
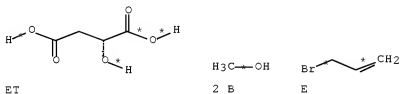
RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

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RX(13) RCT AL 103-80-0, AD 609847-52-1
 PRO AM 609846-41-5
 SOL 110-86-1 Pyridine
 CON 29 hours, room temperature

RX(600) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(14)
 RX(600) ET + 2 B + E + C + AN ==> AO



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)
 RGT D 7719-09-7 SOCl2
 CON room temperature

STAGE(2)
 RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF

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CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4

SOL 7732-18-5 Water, 109-99-9 THF

CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 876-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

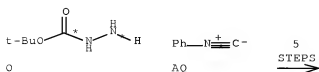
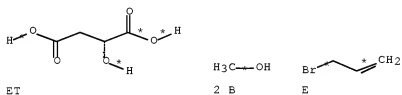
RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

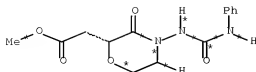
RX(14) RCT AN 1939-99-7, AD 609847-52-1
 PRO AO 609846-42-6
 SOL 110-86-1 Pyridine
 CON 24 hours, room temperature

RX(601) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16)

RX(601) ET + 2 B + E + O + AQ ==> AR



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AR
YIELD 100%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)

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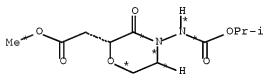
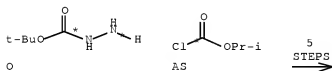
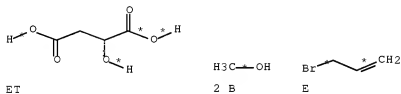
SOL 108-88-3 PhMe
CON 25 hours, room temperature

STAGE(2)

RGT B 67-56-1 MeOH
SOL 67-56-1 MeOH
CON 5 minutes, 40 deg C

PRO AR 609646-44-6

RX(602) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(17)
RX(602) ET + 2 B + E + O + AS ==> AT



AT
YIELD 93%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

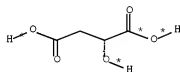
RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

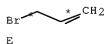
RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(17) RCT AS 108-23-6, AD 609847-52-1
 PRO AT 609846-45-9
 SOL 108-88-3 PhMe, 110-86-1 Pyridine
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 4 hours

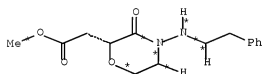
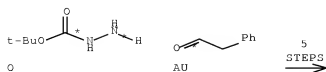
RX(603) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(18)
 RX(603) ET + 2 B + E + C + AU ==> AV



ET



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AV
YIELD 100%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0

RGT R 1333-74-0 H₂

PRO AG 609847-50-9

CAT 7440-05-3 Pd

SOL 109-99-9 THF

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CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(18) RCT AU 122-78-1, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

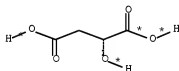
RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 2 hours, room temperature

PRO AV 609846-46-0

RX(604) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(20)

RX(604) 2 ET + 3 B + 2 E + 2 O + 3 AX ==>

AY + AZ



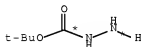
2 ET



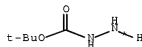
3 B



2 E



O

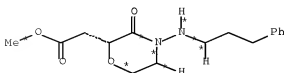


O

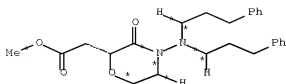


3 AX

5
 STEPS
 →



AY
 YIELD 55%



AZ
YIELD 37%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl₂
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag₂O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO₄
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H₂
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

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RX(20) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)

RGT R 1333-74-0 H2

CAT 7440-05-3 Pd

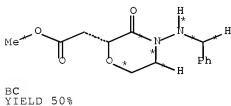
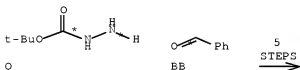
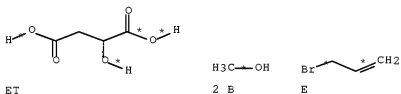
SOL 109-99-9 THF

CON 70 minutes, room temperature

PRO AY 609846-48-2, AZ 609846-49-3

RX(605) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(22)

RX(605) ET + 2 B + E + O + BB ==> BC



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2

CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 876-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(22) RCT BB 100-52-7, AD 609847-52-1

STAGE(1)

RGT BD 1125-88-8 PhCH(OMe)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 80 deg C
SUBSTAGE(2) 2 days, 80 deg C

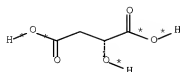
STAGE(2)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 5 minutes, room temperature

PRO BC 609846-51-7

RX(606) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(74)
RX(606) ET + 2 B + E + C + Al + CL + DM ==>
DT

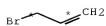
10/595943



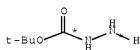
ET



2 B



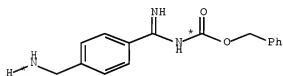
E



O



AI



CL



2 HCl



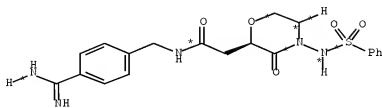
DM



5 STEPS



DT: CM 1
YIELD 29%



DT: CM 2
YIELD 29%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(74) RCT AI 98-09-9, AD 609847-52-1

STAGE(1)

SOL 110-86-1 Pyridine
 CON 20 hours, room temperature

STAGE(2)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

STAGE(4)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2

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SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(5)

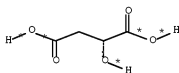
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 80 minutes, room temperature

STAGE(6)

RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO DT 609847-10-1

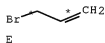
RX(607) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(76)
RX(607) ET + 2 B + E + O + AL + CL + DM ==>
DV



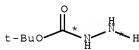
ET



2 B



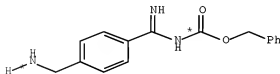
E



O



AL



CL



2

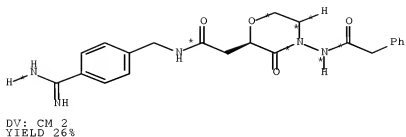
HCl



DM

5
STEPS
→

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
 CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-26-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(76) RCT AL 103-80-0, AD 609847-52-1

STAGE(1)

SOL 110-86-1 Pyridine
CON 29 hours, room temperature

STAGE(2)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(4)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)₂
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(5)

RGT R 1333-74-0 H₂
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 60 minutes, room temperature

STAGE(6)

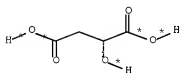
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO DV 699847-14-5

RX(608) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(77)

RX(608) ET + 2 B + E + O + AN + CL + DM ==>

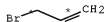
DM



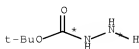
ET



2 B



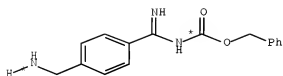
E



O

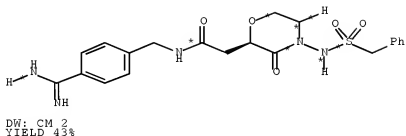


AN



CL

● 2 HCl

5
STEPS
→

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

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RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(77) RCT AN 1939-99-7, AD 609847-52-1

STAGE(1)
SOL 110-86-1 Pyridine
CON 24 hours, room temperature

STAGE(2)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(3)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(4)
RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

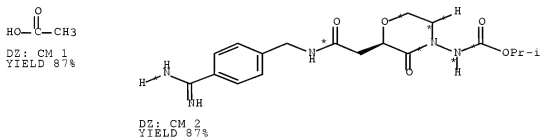
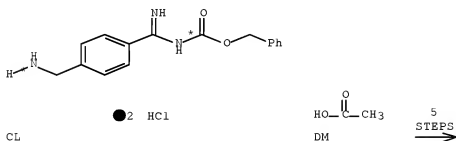
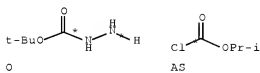
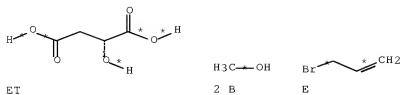
STAGE(5)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 31 hours, room temperature

STAGE(6)
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO DW 609847-16-7

RX(609) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(80)
RX(609) ET + 2 B + E + C + AS + CL + DM ==>
DZ

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RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12

CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

RX(80) RCT AS 108-23-6, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe, 110-86-1 Pyridine
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 4 hours

STAGE(2)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(3)

RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

STAGE(4)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,

10/595943

hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

STAGE(5)

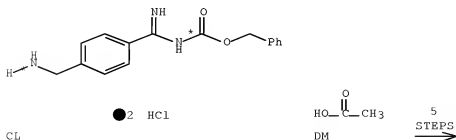
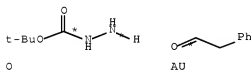
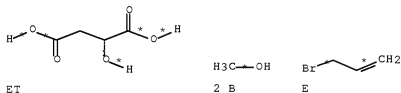
RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 1 hour, room temperature

STAGE(6)

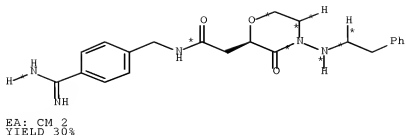
RCT DM 64-19-7
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

PRO DZ 609847-22-5

RX(610) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(81)
 RX(610) ET + 2 B + E + O + AU + CL + DM ==>
 EA



CC(=O)O
 EA: CM 1
 YIELD 30%



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
 CON room temperature

STAGE(2)

RCT E 106-95-6
 RGT G 20667-12-3 Ag2O
 SOL 108-88-3 PhMe
 CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 879-46-2, EU 441764-51-8
 PRO ES 609847-51-0
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
 RGT R 1333-74-0 H2
 PRO AG 609847-50-9
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
 PRO AD 609847-52-1
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

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RX(81) RCT AU 122-78-1, AD 609847-52-1

STAGE(1)

SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, 60 deg C

STAGE(2)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 2 hours, room temperature

STAGE(3)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(4)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

STAGE(5)

RCT CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 80 minutes, room temperature

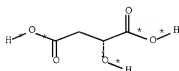
STAGE(7)

RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO EA 609847-24-7

RX(611) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(83)

RX(611) ET + 2 B + E + O + AX + CL + DM ==>
EC



ET

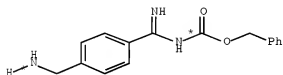
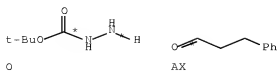


2 B



E

10/595943

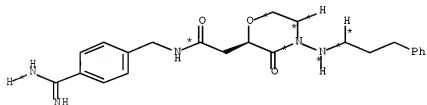


CL

● 2 HCl



5
STEPS
➔



EC: CM 2
 YIELD 49%

RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOCl2
 CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 870-46-2, EU 441764-51-8
PRO ES 609847-51-0
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(83) RCT AX 104-53-0, AD 609847-52-1

STAGE(1)
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 24 hours, 70 deg C

STAGE(2)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 70 minutes, room temperature

STAGE(3)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(4)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

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STAGE(5)

RCT CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

STAGE(6)

RGT R 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 2 hours, room temperature

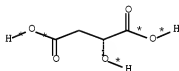
STAGE(7)

RCT DM 64-19-7
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

PRO EC 609847-28-1

RX(612) OF 616 COMPOSED OF RX(95), RX(96), RX(94), RX(97), RX(16), RX(38),
 RX(54), RX(79)

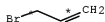
RX(612) ET + 2 B + E + O + AQ + CL + DM ==>
 DY



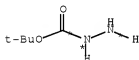
ET



2 B



E

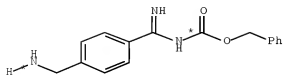


O



AQ

10/595943

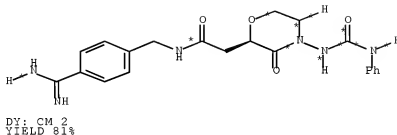


CL

● 2 HCl



8
STEPS
→



RX(95) RCT ET 636-61-3, B 67-56-1

STAGE(1)

RGT D 7719-09-7 SOC12
CON room temperature

STAGE(2)

RCT E 106-95-6
RGT G 20667-12-3 Ag2O
SOL 108-88-3 PhMe
CON room temperature

STAGE(3)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(4)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO EU 441764-51-8

RX(96) RCT O 879-46-2, EU 441764-51-8

PRO ES 609847-51-0

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> 65 deg C

SUBSTAGE(2) overnight, 65 deg C

RX(94) RCT ES 609847-51-0
RGT R 1333-74-0 H2
PRO AG 609847-50-9
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(97) RCT AG 609847-50-9
PRO AD 609847-52-1
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(16) RCT AQ 931-54-4, AD 609847-52-1

STAGE(1)
SOL 108-88-3 PhMe
CON 25 hours, room temperature

STAGE(2)
RGT B 67-56-1 MeOH
SOL 67-56-1 MeOH
CON 5 minutes, 40 deg C

PRO AR 609846-44-8

RX(38) RCT AR 609846-44-8

STAGE(1)
RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)
RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

PRO CF 609846-68-6

RX(54) RCT CF 609846-68-6, CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
PRO CX 609846-84-6
SOL 68-12-2 DMF
CON 100 minutes, room temperature

RX(79) RCT CX 609846-84-6

STAGE(1)
RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 64-17-5 EtOH, 109-99-9 THF
CON 2 hours, room temperature

STAGE(2)
RCT DM 64-19-7
SOL 7732-18-5 Water, 67-56-1 MeOH

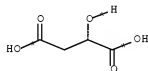
10/595943

CON room temperature

PRO DY 609847-20-3

RX(613) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7),
RX(44), RX(69)

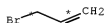
RX(613) A + 2 B + E + O + U + CL + DM ==>
DM



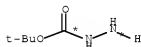
A



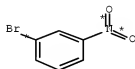
2 B



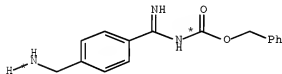
E



O



U



CL

2 HCl



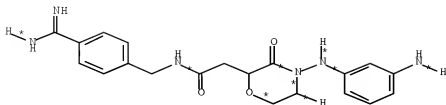
DM

9
STEPS
➔



DN: CM 1
YIELD 48%

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DN: CM 2
YIELD 48%

RX(1) RCT A 97-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)
RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

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```
RX(7)      RCT  T 609846-34-6, U 585-79-5
           RGT  W 534-17-8 Cs2CO3
           PRO  V 609846-35-7
           CAT  161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-
           diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
           SOL  108-88-3 PhMe
           CON  SUBSTAGE(1) room temperature
                SUBSTAGE(2) room temperature -> 95 deg C
                SUBSTAGE(3) 19 hours, 95 deg C

RX(44)     RCT  V 609846-35-7

           STAGE(1)
           RGT  BW 1310-65-2 LiOH
           SOL  7732-18-5 Water, 67-56-1 MeOH
           CON  room temperature

           STAGE(2)
           RGT  BX 7647-01-0 HCl
           SOL  7732-18-5 Water
           CON  room temperature

           STAGE(3)
           RCT  CL 172348-75-3
           RGT  CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
           1-[bis(dimethylamino)methylene]-, 3-oxide,
           hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
           SOL  68-12-2 DMF
           CON  100 minutes, room temperature

           PRO  CM 609846-74-4

RX(69)     RCT  CM 609846-74-4

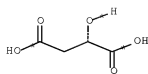
           STAGE(1)
           RGT  R 1333-74-0 H2
           CAT  7440-05-3 Pd
           SOL  7732-18-5 Water, 64-17-5 EtOH
           CON  1 hour, room temperature

           STAGE(2)
           RCT  DM 64-19-7
           SOL  7732-18-5 Water, 67-56-1 MeOH

           PRO  DN 609847-00-9

RX(614) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(8),
RX(31), RX(45)
RX(614) 2 A + 4 B + 2 E + 2 O + 3 Z + CL ==>
CO
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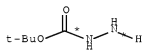
2 A



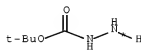
4 B



2 E



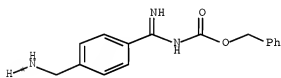
O



O



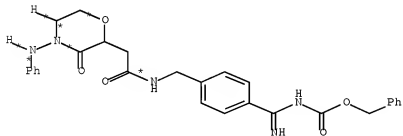
3 Z



CL



9
STEPS
→



CO

RX(1) RCT A 57-67-6, B 67-56-1
RGT D 7719-09-7 SOC12
PRO C 617-55-0
CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6

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RGT G 20667-12-3 Ag2O
PRO F 297749-53-2
SOL 108-88-3 PhMe
CON room temperature
NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)

RGT J 7529-22-8 Me-morpholineoxide
CAT 20816-12-0 OsO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

STAGE(2)

RGT K 7790-28-5 NaIO4
SOL 7732-18-5 Water, 109-99-9 THF
CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
PRO P 609846-32-4
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> 65 deg C
SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(8) RCT T 609846-34-6, Z 108-86-1
RGT W 534-17-8 Cs2CO3
PRO AA 609846-36-8, AB 609847-53-2
CAT 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, 3375-31-3 Pd(OAc)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 95 deg C
SUBSTAGE(3) 19 hours, 95 deg C

RX(31) RCT AB 609847-53-2

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water

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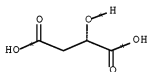
CON room temperature

PRO BY 609846-61-9

RX(45) RCT BY 609846-61-9, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 PRO CO 609846-75-5
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

RX(615) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(12),
 RX(35), RX(50)

RX(615) A + 2 B + E + O + AI + CL ==>
 CT



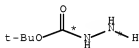
A



2 B



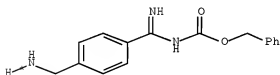
E



O



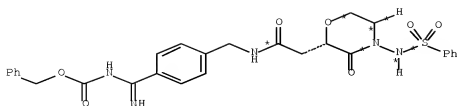
AI



CL

● 2 HCl

9
 STEPS
 →



CT

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOCl2
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 870-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C
 SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
 RGT R 1333-74-0 H2
 PRO Q 609846-33-5
 CAT 7440-05-3 Pd
 SOL 109-99-9 THF
 CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
 PRO T 609846-34-6
 SOL 7732-18-5 Water
 CON 7 hours, 60 deg C
 NTE key intermediate

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RX(12) RCT T 609846-34-6, AI 98-09-9
 PRO AK 609846-40-4
 SOL 110-86-1 Pyridine
 CON 20 hours, room temperature

RX(35) RCT AK 609846-40-4

STAGE(1)

RGT BW 1310-65-2 LiOH
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON room temperature

STAGE(2)

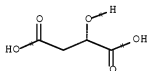
RGT BX 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO CC 609846-65-3

RX(50) RCT CC 609846-65-3, CL 172348-75-3
 RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
 1-[bis(dimethylamino)methylene]-, 3-oxide,
 hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
 PRO CT 609846-80-2
 SOL 68-12-2 DMF
 CON 100 minutes, room temperature

RX(616) OF 616 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(21),
 RX(42), RX(59)

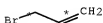
RX(616) A + 2 B + E + O + AX + CL ==>
 DC



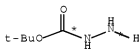
A



2 B



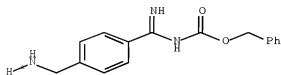
E



O

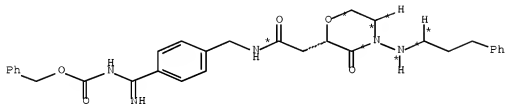


AX



CL

● 2 HCl

 9
 STEPS


DC

RX(1) RCT A 97-67-6, B 67-56-1
 RGT D 7719-09-7 SOC12
 PRO C 617-55-0
 CON room temperature

RX(2) RCT C 617-55-0, E 106-95-6
 RGT G 20667-12-3 Ag2O
 PRO F 297749-53-2
 SOL 108-88-3 PhMe
 CON room temperature
 NTE other product also detected

RX(3) RCT F 297749-53-2

STAGE(1)
 RGT J 7529-22-8 Me-morpholineoxide
 CAT 20816-12-0 OsO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

STAGE(2)
 RGT K 7790-28-5 NaIO4
 SOL 7732-18-5 Water, 109-99-9 THF
 CON room temperature

PRO I 441764-54-1

RX(4) RCT I 441764-54-1, O 970-46-2
 PRO P 609846-32-4
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> 65 deg C

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SUBSTAGE(2) overnight, 65 deg C

RX(5) RCT P 609846-32-4
RGT R 1333-74-0 H2
PRO Q 609846-33-5
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 18 hours, room temperature

RX(6) RCT Q 609846-33-5
PRO T 609846-34-6
SOL 7732-18-5 Water
CON 7 hours, 60 deg C
NTE key intermediate

RX(21) RCT T 609846-34-6, AX 104-53-0

STAGE(1)

SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 5 hours, 70 deg C

STAGE(2)

RGT R 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 3 hours, room temperature

PRO BA 609846-50-6

RX(42) RCT BA 609846-50-6

STAGE(1)

RGT BW 1310-65-2 LiOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

STAGE(2)

RGT BX 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

PRO CJ 609846-72-2

RX(59) RCT CJ 609846-72-2, CL 172348-75-3
RGT CN 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, 3-oxide,
hexafluorophosphate(1-) (1:1), BH 7087-68-5 EtN(Pr-i)2
PRO DC 609846-89-1
SOL 68-12-2 DMF
CON 100 minutes, room temperature

L91 ANSWER 13 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 122:214089 CASREACT Full-text

TITLE: Novel synthesis of
[(tetrazolylbiphenyl)methyl]tetraazacyclopentanaphth
alenone

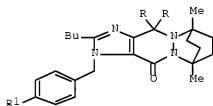
INVENTOR(S): Yamada, Hiroyoshi; Munesada, Kiyotaka; Koh, Keiko;
Tsuzuki, Kazuo; Taniguchi, Mikio; Fujita, Yoshiji

10/595943

PATENT ASSIGNEE(S): Upjohn Co., USA
 SOURCE: PCT Int. Appl., 18 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9500517	A1	19950105	WO 1994-US6028	19940602
W:	AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KG, KP, KR, KZ, LK, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN			
RW:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
JP 07010879	A	19950113	JP 1993-149132	19930621
AU 9470967	A	19950117	AU 1994-70967	19940602
EP 705266	A1	19960410	EP 1994-920047	19940602
EP 705266	B1	19970226		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE			
JP 08512029	T	19961217	JP 1995-502833	19940602
JP 3391402	B2	20030331		
AT 149168	T	19970315	AT 1994-920047	19940602
ES 2099621	T3	19970516	ES 1994-920047	19940602
US 6005105	A	19991221	US 1995-557072	19951206
PRIORITY APPLN. INFO.:			JP 1993-149132	19930621
			WO 1994-US6028	19940602

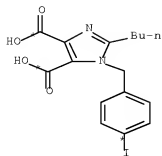
GI



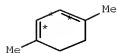
I

AB Halobenzyltetraazacyclopentanaphthalenedione I (RR = O, R1 = iodo)(preparation given) was condensed with 5-phenyl-1-triphenylmethyl-1H-tetrazole to give, after reduction and deprotection, I (R = H, R1 = 2-tetrazol-5-ylphenyl).

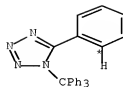
RX(17) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(7)
 RX(17) A + E + Z ==> N



A



E



Z

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N₂H₄

STAGE(2)

RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT G 546-67-8 Pb(OAc)₄

STAGE(3)

SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K 1576-35-8 Tosylhydrazide

SOL 68-12-2 DMF

STAGE(2)

SOL 141-78-6 AcOEt, 7732-18-5 Water

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PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RGT AB 7646-85-7 ZnCl2

SOL 109-99-9 THF

STAGE(3)

RGT AC 676-58-4 MeMgCl

CAT 14264-16-5 NiCl2(PPh3)2

SOL 109-99-9 THF

STAGE(4)

RCT J 161800-12-0

SOL 109-99-9 THF

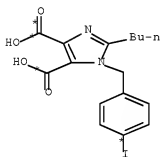
STAGE(5)

RGT AD 64-19-7 AcOH

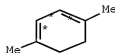
PRO N 161800-13-1

RX(23) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(7), RX(4)

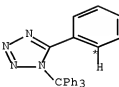
RX(23) A + E + Z ==> O



A



E



Z

5
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

10/595943

RX(1) RCT A 161800-09-5
STAGE(1)
RGT C 302-01-2 N2H4
STAGE(2)
RGT D 7732-18-5 Water
PRO B 161800-10-8
RX(2) RCT B 161800-10-8, E 26120-52-5
STAGE(1)
SOL 75-09-2 CH2Cl2
STAGE(2)
RGT G 546-67-8 Pb(OAc)4
STAGE(3)
SOL 108-88-3 PhMe
PRO F 161800-11-9
RX(3) RCT F 161800-11-9
STAGE(1)
RGT K 1576-35-8 Tosylhydrazide
SOL 68-12-2 DMF
STAGE(2)
SOL 141-78-6 AcOEt, 7732-18-5 Water
PRO J 161800-12-0
RX(7) RCT Z 154750-11-5
STAGE(1)
RGT AA 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
STAGE(2)
RGT AB 7646-85-7 ZnCl2
SOL 109-99-9 THF
STAGE(3)
RGT AC 676-58-4 MeMgCl
CAT 14264-16-5 NiCl2(PPh3)2
SOL 109-99-9 THF
STAGE(4)
RCT J 161800-12-0
SOL 109-99-9 THF
STAGE(5)
RGT AD 64-19-7 AcOH
PRO N 161800-13-1
RX(4) RCT N 161800-13-1

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STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT P 1191-15-7 $\text{AlH}(\text{Bu-i})_2$

SOL 108-88-3 PhMe

STAGE(3)

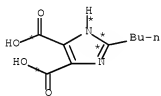
RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

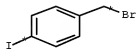
PRO O 161800-14-2

RX(24) OF 28 COMPOSED OF RX(6), RX(1), RX(2), RX(3), RX(7)

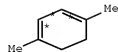
RX(24) V + W + E + Z ==> N



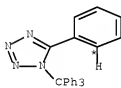
V



W

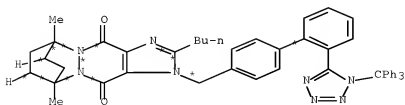


E



Z

5
STEPS
→



N
YIELD 77%

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RX(6) RCT V 71998-99-7, W 16004-15-2

STAGE(1)

RGT X 7646-69-7 NaH

SOL 68-12-2 DMF

STAGE(2)

RGT Y 67-56-1 MeOH

PRO A 161800-09-5

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 362-01-2 N2H4

STAGE(2)

RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT G 546-67-8 Pb(OAc)4

STAGE(3)

SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K 1576-35-8 Tosylhydrazide

SOL 68-12-2 DMF

STAGE(2)

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RGT AB 7646-69-7 ZnCl2

SOL 109-99-9 THF

STAGE(3)

RGT AC 676-58-4 MeMgCl

CAT 14264-16-5 NiCl2(PPh3)2

SOL 109-99-9 THF

10/595943

STAGE(4)

RCT J 161800-12-0

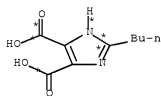
SOL 109-99-9 THF

STAGE(5)

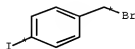
RGT AD 64-19-7 AcOH

PRO N 161800-13-1

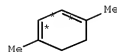
RX(25) OF 28 COMPOSED OF RX(6), RX(1), RX(2), RX(3), RX(7), RX(4)
 RX(25) V + W + E + Z ==> O



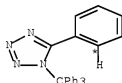
V



W

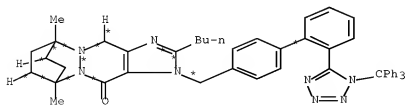


E



Z

6
STEPS
→



O
YIELD 97%

RX(6) RCT V 71598-99-7, W 16004-15-2

STAGE(1)
RGT X 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RGT Y 67-56-1 MeOH

PRO A 161800-09-5

RX(1) RCT A 161800-09-5

STAGE(1)
RGT C 302-01-2 N2H4

STAGE(2)
RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT G 546-67-8 Pb(OAc)4

STAGE(3)
SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)
RGT K 1576-35-8 Tosylhydrazide
SOL 68-12-2 DMF

STAGE(2)
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)
RGT AA 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)
RGT AB 7646-85-7 ZnCl2
SOL 109-99-9 THF

STAGE(3)
RGT AC 676-58-4 MeMgCl
CAT 14264-16-5 NiCl2(PPh3)2
SOL 109-99-9 THF

STAGE(4)
RCT J 161800-12-0

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SOL 109-99-9 THF

STAGE(5)

RGT AD 64-19-7 AcOH

PRO N 161800-13-1

RX(4) RCT N 161800-13-1

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT P 1191-15-7 AlH(Bu-i)2

SOL 108-88-3 PhMe

STAGE(3)

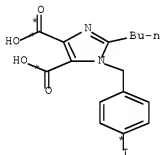
RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

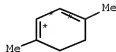
PRO O 161800-14-2

RX(27) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(7), RX(4), RX(5)

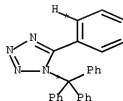
RX(27) A + E + Z ==> S



A



E



Z



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N2H4

STAGE(2)
RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT G 546-67-8 Pb(OAc)4

STAGE(3)
SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)
RGT K 1576-35-8 Tosylhydrazide
SOL 68-12-2 DMF

STAGE(2)
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO J 161800-12-0

RX(7) RCT Z 154750-11-5

STAGE(1)
RGT AA 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)
RGT AB 7646-85-7 ZnCl2
SOL 109-99-9 THF

STAGE(3)
RGT AC 676-58-4 MeMgCl
CAT 14264-16-5 NiCl2(PPh3)2
SOL 109-99-9 THF

STAGE(4)
RCT J 161800-12-0
SOL 109-99-9 THF

STAGE(5)
RGT AD 64-19-7 AcOH

PRO N 161800-13-1

RX(4) RCT N 161800-13-1

STAGE(1)
SOL 109-99-9 THF

STAGE(2)
RGT P 1191-15-7 AlH(Bu-i)2

10/595943

SOL 108-88-3 PhMe

STAGE(3)

RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

PRO O 161800-14-2

RX(5) RCT O 161800-14-2

STAGE(1)

RGT T 7647-01-0 HCl

SOL 67-64-1 Me2CO

STAGE(2)

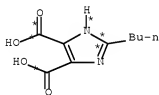
RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

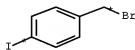
PRO S 152134-03-7

RX(28) OF 28 COMPOSED OF RX(6), RX(1), RX(2), RX(3), RX(7), RX(4), RX(5)

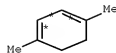
RX(28) V + W + E + Z ==> S



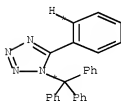
V



W



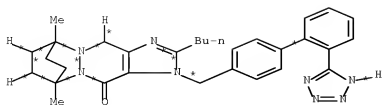
E



Z

7
STEPS
→

10/595943



S
YIELD 91%

RX(6) RCT V 71998-99-7, W 16004-15-2

STAGE(1)

RGT X 7646-69-7 NaH

SOL 68-12-2 DMF

STAGE(2)

RGT Y 67-56-1 MeOH

PRO A 161800-09-5

RX(1) RCT A 161800-09-5

STAGE(1)

RGT C 302-01-2 N2H4

STAGE(2)

RGT D 7732-18-5 Water

PRO B 161800-10-8

RX(2) RCT B 161800-10-8, E 26120-52-5

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT G 546-67-8 Pb(OAc)4

STAGE(3)

SOL 108-88-3 PhMe

PRO F 161800-11-9

RX(3) RCT F 161800-11-9

STAGE(1)

RGT K 1576-35-8 Tosylhydrazide

SOL 68-12-2 DMF

STAGE(2)

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO J 161800-12-0

10/595943

RX(7) RCT Z 154750-11-5

STAGE(1)

RGT AA 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RGT AB 7646-85-7 ZnCl2

SOL 109-99-9 THF

STAGE(3)

RGT AC 676-58-4 MeMgCl

CAT 14264-16-5 NiCl2(PPh3)2

SOL 109-99-9 THF

STAGE(4)

RCT J 161800-12-0

SOL 109-99-9 THF

STAGE(5)

RGT AD 64-19-7 AcOH

PRO N 161800-13-1

RX(4) RCT N 161800-13-1

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT P 1191-15-7 AlH(Bu-i)2

SOL 108-88-3 PhMe

STAGE(3)

RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

PRO O 161800-14-2

RX(5) RCT O 161800-14-2

STAGE(1)

RGT T 7647-01-0 HCl

SOL 67-64-1 Me2CO

STAGE(2)

RGT Q 7647-14-5 NaCl

SOL 7732-18-5 Water

PRO S 152134-03-7

L91 ANSWER 14 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

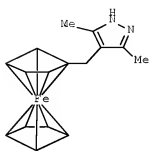
ACCESSION NUMBER: 122:106074 CASREACT [Full-text](#)

TITLE: Ferrocenes and ferrocenophanes with dipolar structure elements

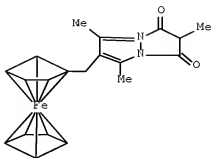
AUTHOR(S): Pagel, Karsten; Werner, Andreas; Friedrichsen, Willy

CORPORATE SOURCE: Institut fuer Organische Chemie der Universitaet Kiel, Olshausenstrasse 40-60, Kiel, D-24018, Germany

SOURCE: Journal of Organometallic Chemistry (1994), 481(1),



I

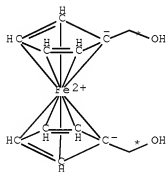


II

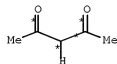
AB The synthesis of ferrocenyl substituted pyrazoles, e.g. I, and the subsequent reaction of these compds. with reactive malonic acid derivs. yielding dipolaric pyrazolo[1,2-a]pyrazol-4-ium-3-olates, e.g. II, is described.

RX(87) OF 260 COMPOSED OF RX(4), RX(5), RX(21)

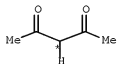
RX(87) L + 2 M + 2 A_Q ==> AB



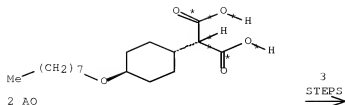
L



M



M



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT L 1291-48-1, M 123-54-6
 RGT O 16872-11-0 HBF₄
 PRO N 160791-68-4
 SOL 7732-18-5 Water

RX(5) RCT N 160791-68-4
 RGT F 302-01-2 N₂H₄
 PRO Q 160791-69-5
 SOL 64-17-5 EtOH

RX(21) RCT AQ 123654-20-6

STAGE(1)
 RGT AS 7719-09-7 SOCl₂

STAGE(2)
 SOL 109-99-9 THF

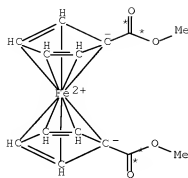
STAGE(3)
 RCT Q 160791-69-5
 SOL 109-99-9 THF

STAGE(4)
 RGT J 121-44-8 Et₃N
 SOL 109-99-9 THF

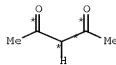
PRO AU 160824-73-7

RX(90) OF 260 COMPOSED OF RX(9), RX(4), RX(5), RX(21)

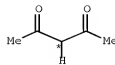
RX(90) AD + 2 M + 2 AQ ==> AU



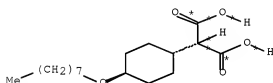
AD



M



M



2 AQ

4
STEPS
➔

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(9) RCT AD 1273-95-6
RGT AB 16853-85-3 LiAlH4
PRO L 1291-48-1
SOL 109-99-9 THF

RX(4) RCT L 1291-48-1, M 123-54-6
RGT O 16872-11-0 HBF4
PRO N 160791-68-4
SOL 7732-18-5 Water

RX(5) RCT N 160791-68-4
RGT F 302-01-2 N2H4
PRO Q 160791-69-5
SOL 64-17-5 EtOH

RX(21) RCT AQ 123854-26-6

STAGE(1)
RGT AS 7719-09-7 SOCl2

STAGE(2)
SOL 109-99-9 THF

STAGE(3)
RCT Q 160791-69-5

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SOL 109-99-9 THF

STAGE(4)

RGT J 121-44-8 Et3N

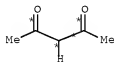
SOL 109-99-9 THF

PRO AU 160824-73-7

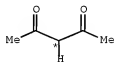
RX(101) OF 260 COMPOSED OF RX(11), RX(13), RX(22)

RX(101) AE + 2 M + 2 AV ==> AW

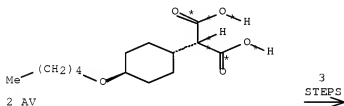
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



M



M



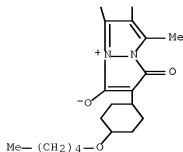
2 AV

3
STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



Me-(CH2)4-O

AW
YIELD 43%

10/595943

RX(11) RCT AE 108693-71-6, M 123-54-6
 RGT O 16872-11-0 HBF4
 PRO AF 160791-70-8
 SOL 75-09-2 CH2Cl2
 NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8
 RGT F 302-01-2 N2H4
 PRO AH 160791-72-0
 SOL 64-17-5 EtOH

RX(22) RCT AV 160811-27-8

STAGE(1)
 RGT AS 7719-09-7 SOCl2

STAGE(2)
 SOL 109-99-9 THF

STAGE(3)
 RCT AH 160791-72-0
 SOL 109-99-9 THF

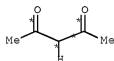
STAGE(4)
 RGT J 121-44-8 Et3N
 SOL 109-99-9 THF

PRO AW 160791-75-3

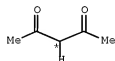
RX(102) OF 260 COMPOSED OF RX(11), RX(13), RX(24)

RX(102) AE + 2 M + 2 AQ ==> AY

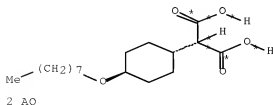
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



M



M



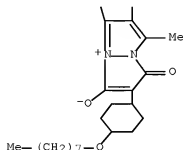
2 AQ

3
 STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A

AY
YIELD 59%

RX(11) RCT AE 108693-71-6, M 123-54-6
 RGT O 16872-11-0 HBF₄
 PRO AF 160791-70-8
 SOL 75-09-2 CH₂Cl₂
 NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8
 RGT F 302-01-2 N₂H₄
 PRO AH 160791-72-0
 SOL 64-17-5 EtOH

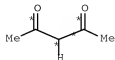
RX(24) RCT AQ 123854-20-6
 STAGE(1)
 RGT AS 7719-09-7 SOCl₂
 STAGE(2)
 SOL 109-99-9 THF
 STAGE(3)
 RCT AH 160791-72-0
 SOL 109-99-9 THF
 STAGE(4)
 RGT J 121-44-8 Et₃N
 SOL 109-99-9 THF

PRO AY 160791-77-5

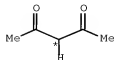
RX(103) OF 260 COMPOSED OF RX(10), RX(11), RX(13), RX(22)
 RX(103) W + 2 M + 2 AY ==> AH

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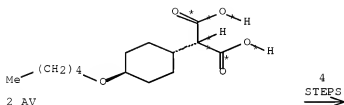
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



M



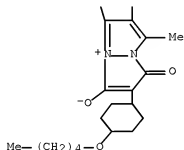
M



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



AW
YIELD 43%

RX(10) RCT W 82522-10-9
RGT AB 16853-85-3 LiAlH4
PRO AE 108693-71-6
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6
RGT O 16872-11-0 HBF4
PRO AF 160791-70-8
SOL 75-09-2 CH2Cl2

10/595943

NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8
 RGT F 302-01-2 N2H4
 PRO AH 160791-72-0
 SOL 64-17-5 EtOH

RX(22) RCT AV 160811-27-8

STAGE(1)
 RGT AS 7719-09-7 SOC12

STAGE(2)
 SOL 109-99-9 THF

STAGE(3)
 RCT AH 160791-72-0
 SOL 109-99-9 THF

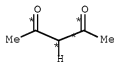
STAGE(4)
 RGT J 121-44-8 Et3N
 SOL 109-99-9 THF

PRO AW 160791-75-3

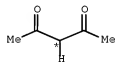
RX(104) OF 260 COMPOSED OF RX(10), RX(11), RX(13), RX(24)

RX(104) W + 2 M + 2 AQ ==> AY

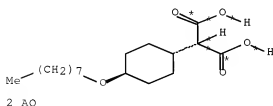
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



M



M

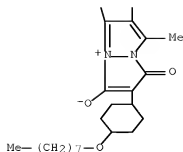


2 AQ

4
 STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



AY
YIELD 59%

RX(10) RCT W 82522-10-9
RGT AB 16853-85-3 LiAlH₄
PRO AE 108693-71-6
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6
RGT O 16872-11-0 HBF₄
PRO AF 160791-70-8
SOL 75-09-2 CH₂Cl₂
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8
RGT F 302-01-2 N₂H₄
PRO AH 160791-72-0
SOL 64-17-5 EtOH

RX(24) RCT AQ 123654-20-6

STAGE(1)
RGT AS 7719-09-7 SOCl₂

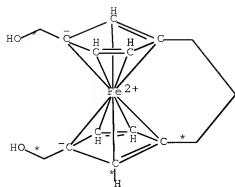
STAGE(2)
SOL 109-99-9 THF

STAGE(3)
RCT AH 160791-72-0
SOL 109-99-9 THF

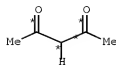
STAGE(4)
RGT J 121-44-8 Et₃N
SOL 109-99-9 THF

PRO AY 160791-77-5

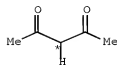
RX(105) OF 260 COMPOSED OF RX(12), RX(14), RX(23)
RX(105) AA + 2 M + 2 AV ==> AX



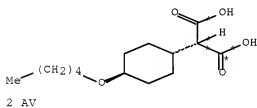
AA



M



M

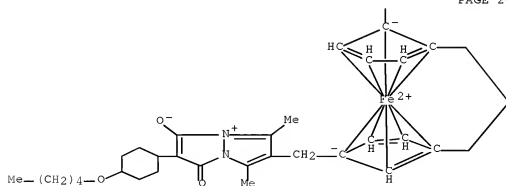


2 AV

3
STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



AX
YIELD 38%

RX(12) RCT AA 108693-72-7, M 123-54-6
RGT O 16372-11-0 HBF4
PRO AG 160791-71-9

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SOL 75-09-2 CH2C12

RX(14) RCT AG 160791-71-9
 RGT F 302-01-2 N2H4
 PRO AI 160824-68-0
 SOL 64-17-5 EtOH

RX(23) RCT AV 160811-27-8

STAGE(1)
 RGT AS 7719-09-7 SOC12

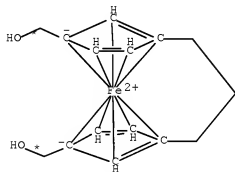
STAGE(2)
 SOL 109-99-9 THF

STAGE(3)
 RCT AI 160824-68-0
 SOL 109-99-9 THF

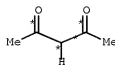
STAGE(4)
 RGT J 121-44-8 Et3N
 SOL 109-99-9 THF

PRO AX 160791-76-4

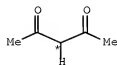
RX(106) OF 260 COMPOSED OF RX(12), RX(14), RX(25)
 RX(106) AA + 2 M + 2 AQ ==> AZ



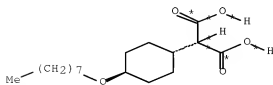
AA



M



M



2 AQ

3
 STEPS
 ➔

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(12) RCT AA 108693-72-7, M 123-54-6
 RGT O 16872-11-0 HBF₄
 PRO AG 160791-71-9
 SOL 75-09-2 CH₂Cl₂

RX(14) RCT AG 160791-71-9
 RGT F 302-01-2 N₂H₄
 PRO AI 160824-68-0
 SOL 64-17-5 EtOH

RX(25) RCT AQ 123854-20-6

STAGE(1)
 RGT AS 7719-09-7 SOCl₂

STAGE(2)
 SOL 109-99-9 THF

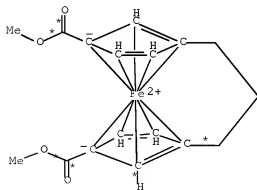
STAGE(3)
 RCT AI 160824-68-0
 SOL 109-99-9 THF

STAGE(4)
 RGT J 121-44-8 Et₃N
 SOL 109-99-9 THF

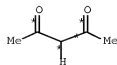
PRO AZ 160791-70-6

RX(107) OF 260 COMPOSED OF RX(8), RX(12), RX(14), RX(23)

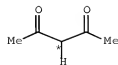
RX(107) X + 2 M + 2 AV ==> AX



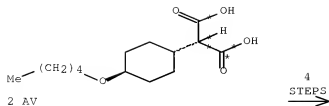
X



M

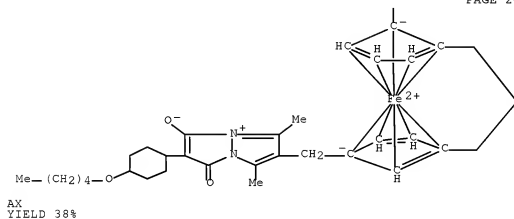


M



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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RX(8)	RCT	X 82544-17-0
	RGT	AB 16853-85-3 LiAlH4
	PRO	AA 108693-72-7
	SOL	109-99-9 THF
RX(12)	RCT	AA 108693-72-7, M 123-54-6
	RGT	O 16872-11-0 HBF4
	PRO	AG 160791-71-9
	SOL	75-09-2 CH2Cl2
RX(14)	RCT	AG 160791-71-9
	RGT	F 302-01-2 N2H4
	PRO	AI 160824-68-0
	SOL	64-17-5 EtOH
RX(23)	RCT	AV 160811-27-8
	STAGE(1)	
	RGT	AS 7719-09-7 SOCl2
	STAGE(2)	
	SOL	109-99-9 THF

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STAGE(3)

RCT AI 160824-68-0

SOL 109-99-9 THF

STAGE(4)

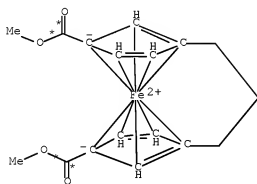
RGT J 121-44-8 Et3N

SOL 109-99-9 THF

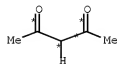
PRO AX 160791-76-4

RX(108) OF 260 COMPOSED OF RX(8), RX(12), RX(14), RX(25)

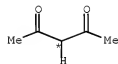
RX(108) X + 2 M + 2 AQ ==> AZ



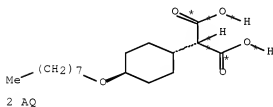
X



M



M



2 AQ

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(8)

RCT X 82544-17-0

RGT AB 16853-85-3 LiAlH4

PRO AA 108693-72-7

SOL 109-99-9 THF

RX(12)

RCT AA 108693-72-7, M 123-54-6

RGT O 16872-11-0 HBF4

PRO AG 160791-71-9

SOL 75-09-2 CH2Cl2

10/595943

RX(14) RCT AG 160791-71-9
 RGT F 302-01-2 N2H4
 PRO AI 160824-68-0
 SOL 64-17-5 EtOH

RX(25) RCT AQ 123054-20-6

STAGE(1)
 RGT AS 7719-09-7 SOC12

STAGE(2)
 SOL 109-99-9 THF

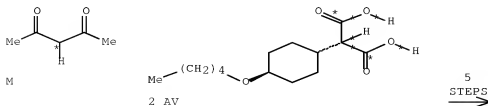
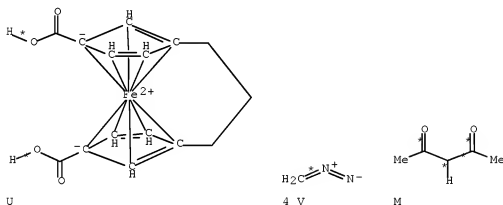
STAGE(3)
 RCT AI 160824-68-0
 SOL 109-99-9 THF

STAGE(4)
 RGT J 121-44-8 Et3N
 SOL 109-99-9 THF

PRO AZ 160791-70-6

RX(160) OF 260 COMPOSED OF RX(7), RX(10), RX(11), RX(13), RX(22)
 RX(160) T + U + 4 V + 2 M + 2 AV ==> AW

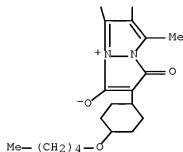
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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AW
YIELD 43%

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3
PRO W 82522-10-9, X 82544-17-0
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(10) RCT W 82522-10-9
RGT AB 16853-85-3 LiAlH4
PRO AE 108693-71-6
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6
RGT O 16872-11-0 HBF4
PRO AF 160791-70-8
SOL 75-09-2 CH2Cl2
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8
RGT F 302-01-2 NH4
PRO AH 160791-72-0
SOL 64-17-5 EtOH

RX(22) RCT AV 160811-27-8

STAGE(1)
RGT AS 7719-09-7 SOCl2

STAGE(2)
SOL 109-99-9 THF

STAGE(3)
RCT AH 160791-72-0
SOL 109-99-9 THF

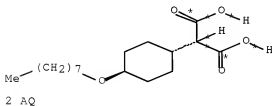
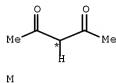
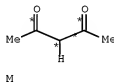
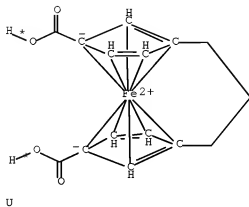
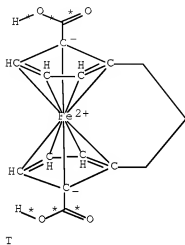
STAGE(4)
RGT J 121-44-8 Et3N

10/595943

SOL 109-99-9 THF

PRO AW 160791-75-3

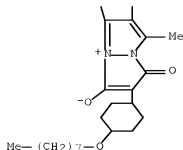
RX(161) OF 260 COMPOSED OF RX(7), RX(10), RX(11), RX(13), RX(24)
 RX(161) T + U + 4 V + 2 M + 2 AQ ==> AT



5
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



AY
YIELD 59%

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3
PRO W 82522-10-9, X 82544-17-0
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(10) RCT W 82522-10-9
RGT AB 16853-85-3 LiAlH₄
PRO AE 108693-71-6
SOL 109-99-9 THF

RX(11) RCT AE 108693-71-6, M 123-54-6
RGT O 16672-11-0 HBF₄
PRO AF 160791-70-8
SOL 75-09-2 CH₂Cl₂
NTE (16% CRYSTALS, 46% OIL)

RX(13) RCT AF 160791-70-8
RGT F 302-01-2 N₂H₄
PRO AH 160791-72-0
SOL 64-17-5 EtOH

RX(24) RCT AQ 123854-20-6

STAGE(1)
RGT AS 7719-09-7 SOCl₂

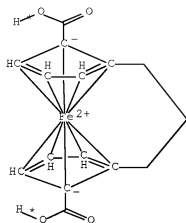
STAGE(2)
SOL 109-99-9 THF

STAGE(3)
RCT AH 160791-72-0
SOL 109-99-9 THF

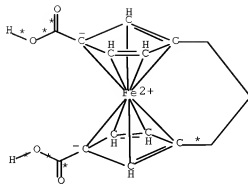
STAGE(4)
RGT J 121-44-8 Et₃N
SOL 109-99-9 THF

PRO AY 160791-77-5

RX(162) OF 260 COMPOSED OF RX(7), RX(8), RX(12), RX(14), RX(23)
RX(162) T + U + 4 V + 2 M + 2 AY ==> AY



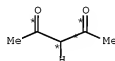
T



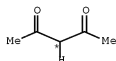
U



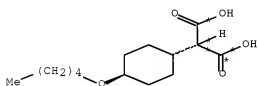
4 V



M



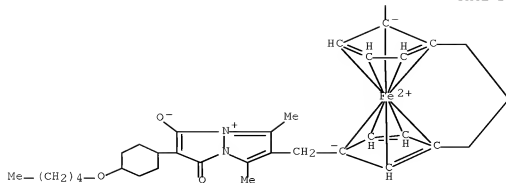
M



2 AV

5
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



AX
YIELD 38%

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3
PRO W 82522-10-9, X 82544-17-0
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(8) RCT X 82544-17-0
RGT AB 16853-85-3 LiAlH4
PRO AA 108693-72-7
SOL 109-99-9 THF

RX(12) RCT AA 108693-72-7, M 123-54-6
RGT O 16872-11-0 HBF4
PRO AG 160791-71-9
SOL 75-09-2 CH2Cl2

RX(14) RCT AG 160791-71-9
RGT F 302-01-2 N2H4
PRO AI 160824-68-0
SOL 64-17-5 EtOH

RX(23) RCT AV 160811-27-8

STAGE (1)
RGT AS 7719-09-7 SOC12

STAGE (2)
SOL 109-99-9 THF

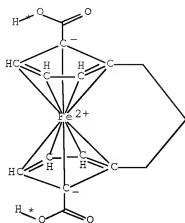
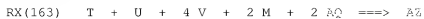
STAGE (3)
RCT AI 160824-68-0
SOL 109-99-9 THF

STAGE (4)
RGT J 121-44-8 Et3N
SOL 109-99-9 THF

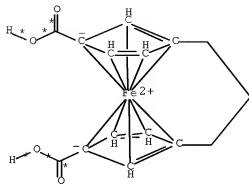
PRO AX 160791-76-4

RX(163) OF 260 COMPOSED OF RX(7), RX(8), RX(12), RX(14), RX(25)

10/595943



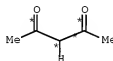
T



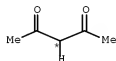
U



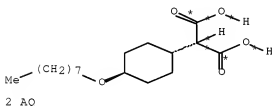
4 V



M



M



2 AQ



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(7) RCT T 155565-57-4, U 155565-58-5, V 334-88-3
 PRO W 82522-10-9, X 82544-17-0
 SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(8) RCT X 82544-17-0
 RGT AB 16853-85-3 LiAlH4
 PRO AA 108693-72-7
 SOL 109-99-9 THF

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RX(12) RCT AA 108693-72-7, M 123-54-6
 RGT O 16872-11-6 HBF₄
 PRO AG 160791-71-9
 SOL 75-09-2 CH₂Cl₂

RX(14) RCT AG 160791-71-9
 RGT F 302-01-2 N₂H₄
 PRO AI 160824-68-0
 SOL 64-17-5 EtOH

RX(25) RCT AQ 123854-20-6

STAGE(1)
 RGT AS 7719-09-7 SOCl₂

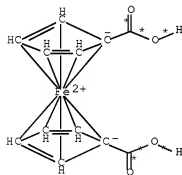
STAGE(2)
 SOL 109-99-9 THF

STAGE(3)
 RCT AI 160824-68-0
 SOL 109-99-9 THF

STAGE(4)
 RGT J 121-44-8 Et₃N
 SOL 109-99-9 THF

PRO AZ 160791-78-6

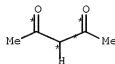
RX(170) OF 260 COMPOSED OF RX(38), RX(9), RX(4), RX(5), RX(21)
 RX(170) CC + 2 V + 2 M + 2 AQ ==> AU



CC

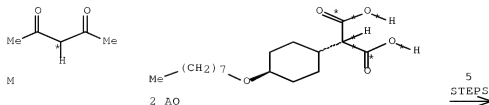


2 V



M

10/595943



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(38) RCT CC 1293-87-4, V 334-88-3
PRO AD 1273-95-6
SOL 67-56-1 MeOH, 60-29-7 Et2O

RX(9) RCT AD 1273-95-6
RGT AB 16853-85-3 LiAlH₄
PRO L 1291-48-1
SOL 109-99-9 THF

RX(4) RCT L 1291-48-1, M 123-54-6
RGT O 16872-11-0 HBF₄
PRO N 160791-68-4
SOL 7732-18-5 Water

RX(5) RCT N 160791-68-4
RGT F 302-01-2 N₂H₄
PRO Q 160791-69-5
SOL 64-17-5 EtOH

RX(21) RCT AQ 123854-20-6

STAGE(1)
RGT AS 7719-09-7 SOCl₂

STAGE(2)
SOL 109-99-9 THF

STAGE(3)
RCT Q 160791-69-5
SOL 109-99-9 THF

STAGE(4)
RGT J 121-44-8 Et₃N
SOL 109-99-9 THF

PRO AU 160824-73-7

L91 ANSWER 15 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 121:83144 CASREACT [Full-text](#)

TITLE: Studies on spiroheterocycles: Synthesis of new spiro-4-thiazolidinones as possible biodynamics

AUTHOR(S): Upadhyay, P.S.; Joshi, H.D.; Baxi, A.J.

CORPORATE SOURCE: Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India

10/595943

SOURCE:

Journal of Sciences, Islamic Republic of Iran (1992),
3(1-2), 30-3

CODEN: JSIIEN; ISSN: 1016-1104

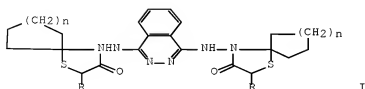
DOCUMENT TYPE:

Journal

LANGUAGE:

English

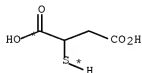
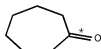
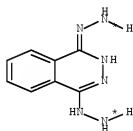
GI



AB Spiro-4-thiazolidinones I ($R = H, Me, CH_2CO_2H, n = 1, 2, 3, 4$) have been synthesized by the cyclocondensation of phthalazinyll hydrazones with cyclic ketones and substituted mercaptoacetic acids, $H_2SCHRCO_2H$. Comps. were screened for their antibacterial, antifungal and antihypertensive activity. The combined elemental analyses and spectroscopic data prove the authenticity of the synthesized compds.

RX(8) OF 8 COMPOSED OF RX(2), RX(5)

RX(8) A + 2 E + 2 L ==> M



2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

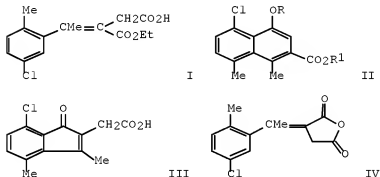
RX(2) RCT A 484-23-1, E 502-42-1
PRO F 156213-51-3
SOL 64-17-5 EtOH

RX(5) RCT F 156213-51-3, L 70-49-5
RGT I 7646-85-7 ZnCl2
PRO M 156213-63-7
NTE thermal

L91 ANSWER 16 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 121:34970 CASREACT [Full-text](#)

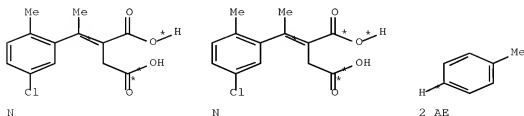
TITLE: The cyclization of (Z)- and (E)-3-ethoxycarbonyl-4-(3'-chloro-6'-methylphenyl)-but-3-enoic acid and synthesis of polysubstituted naphthoic acid
 Mahmoud, M. R.
 Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Journal of the Chemical Society of Pakistan (1993), 15(4), 247-51
 CODEN: JCSPDF; ISSN: 0253-5106
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



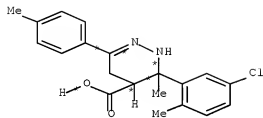
AB Condensing 5-chloro-2-methylacetophenone with di-Et succinate in the presence of KOBu-t (Z)- and (E)-butenoate I. Cyclization of I with Ac₂O gave naphthalene II (R = Ac, H, Me; R₁ = H, Me, Et) and oxoindenyl acid III via the anhydride IV, resp. The reactions of (E)-IV with aromatic hydrocarbons, amines and anhydrous AlCl₃ in Cl₂CHCHCl₂ were also investigated.

RX(54) OF 62 COMPOSED OF RX(5), RX(12), RX(14)

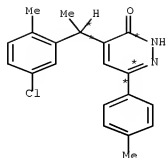
RX(54) 2 N + 2 AE ==> AI + AJ



3
STEPS
→



AI



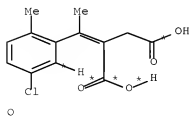
AJ

RX(5) RCT N 155651-98-2
 RGT R 538-75-0 DCC
 PRO J 155651-96-0
 SOL 71-43-2 Benzene

RX(12) RCT J 155651-96-0, AE 108-88-3
 RGT L 7446-70-0 AlCl3
 PRO AF 155652-05-4
 SOL 108-88-3 PhMe

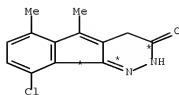
RX(14) RCT AF 155652-05-4
 RGT AK 302-01-2 N2H4
 PRO AI 155652-07-6, AJ 155652-06-7
 SOL 71-36-3 BuOH

RX(56) OF 62 COMPOSED OF RX(6), RX(15), RX(16)
 RX(56) O ==> AN



O

3
STEPS
→



AN

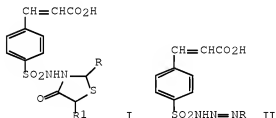
RX(6) RCT O 155651-99-3
 RGT U 75-36-5 AcCl
 PRO T 155652-09-8

RX(15) RCT T 155652-09-8
 RGT L 7446-70-0 AlCl3
 PRO AM 155652-10-1
 SOL 79-34-5 Cl2HCCl2

RX(16) RCT AM 155652-10-1
 RGT AK 302-01-2 N2H4
 PRO AN 155652-12-3
 SOL 71-36-3 BuOH

L91 ANSWER 17 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 117:251263 CASREACT [Full-text](#)
 TITLE: Preparation and antimicrobial activity of
 4-(2'-aryl-5'-H/methyl/carboxymethyl-4'-thiazolidinon-
 3'-yl-aminosulfonyl)cinnamic acids
 AUTHOR(S): Shah, K. C.; Baxi, A. J.
 CORPORATE SOURCE: Dep. Chem., Saurashtra Univ., Rajkot, 360005, India
 SOURCE: Indian Journal of Heterocyclic Chemistry (1992), 1(5),
 253-8
 CODEN: IJCHEI; ISSN: 0971-1627
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

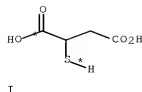
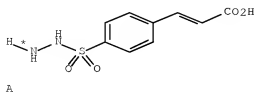


AB Title compds. I [R = Ph, p-(Me2N)C6H4, p-MeOC6H4, p-HOC6H4, o-HOC6H4, cinnamyl, 4-hydroxy-3-methoxyphenyl, 4-H2NC6H4, 3,4-dihydroxyphenyl, 2,4-dichlorophenyl, p-ClC6H4, 2,6-dichlorophenyl, m-O2NC6H4, o-MeOC6H4, m-MeOC6H4, o-ClC6H4, o-O2NC6H4, 3-H2NC6H4, 3,4-dichlorophenyl, 2-hydroxynaphthyl; R1 = H, Me, CH2CO2H] were prepared by the addition condensation of 4-benzalhydrazinosulfonylcinnamic acid II with thioglycolic acid, 2-mercaptopropionic acid and 2-mercaptosuccinic acid. The structures of the compds. have been confirmed by elemental analyses and spectral studies. The products have been screened for their antimicrobial activity.

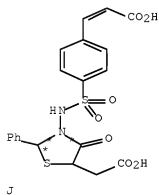
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RX(7) OF 7 COMPOSED OF RX(1), RX(4)

RX(7) A + B + I ==> J



2
STEPS
→



RX(1) RCT A 17641-31-5, B 100-52-7
PRO C 143876-46-4
SOL 123-91-1 Dioxane

RX(4) RCT C 143876-46-4, I 70-49-5
RGT K 7646-85-7 ZnCl2
PRO J 143877-02-5

L91 ANSWER 18 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 113:23664 CASREACT [Full-text](#)
TITLE: Benzophenanthridines. XI. Rodionov-Suvorov systems.
Synthesis of the first example of
11-aminobenzo[c]phenanthridines -
11-amino-6-methyl-11,12-dihydrobenzo[c]phenanthridine

AUTHOR(S): Maslennikova, L. V.; Sladkov, V. I.; Suvorov, N. N.
CORPORATE SOURCE: USSR

10/595943

SOURCE:

Zhurnal Organicheskoi Khimii (1990), 26(2), 441-5

CODEN: ZORKAE; ISSN: 0514-7492

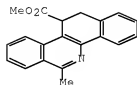
DOCUMENT TYPE:

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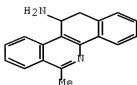
LANGUAGE:

Russian

GI



I

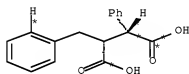


II

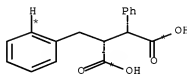
AB Me 6-methyl-11,12-dihydrobenzo[c]phenanthridine-11-carboxylate (I) was prepared from tri-Et 1,3-diphenyl-1,2,2-propanetricarboxylate via formation of erythro-1,3-diphenyl-1,2-propanedicarboxylic acid according to the AD \rightarrow C \rightarrow B Rodionov-Suvorov scheme in an 18% overall yield. Subsequent transformation of I to its hydrazide, azide, and isocyanate followed by Curtius rearrangement gave the title compound II.

RX(38) OF 55 COMPOSED OF RX(3), RX(2), RX(4), RX(5), RX(6), RX(7)

RX(38) 3 B + 3 O ==> V



B



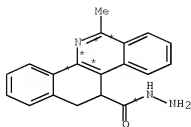
2 B



3 O

6
STEPS
 \longrightarrow

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YIELD 60%

RX(3) RCT B 56906-50-0
 RGT I 334-88-3 CH2N2
 PRO G 20972-45-6
 SOL 60-29-7 Et2O

RX(2) RCT G 20972-45-6
 PRO H 127845-14-1
 NTE polyphosphoric acid

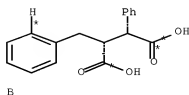
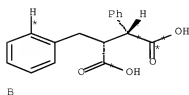
RX(4) RCT H 127845-14-1
 RGT M 5470-11-1 H2NOH-HCl
 PRO K 127845-15-2, L 127845-22-1
 SOL 110-86-1 Pyridine

RX(5) RCT K 127845-15-2, O 108-24-7
 RGT R 7772-99-8 SnCl2
 PRO P 127845-16-3, Q 127845-17-4
 SOL 108-24-7 Ac2O

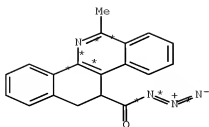
RX(6) RCT Q 127845-17-4
 RGT T 10025-87-3 POC13
 PRO S 104958-38-5
 SOL 95-47-6 o-Xylene

RX(7) RCT S 104958-38-5
 RGT W 302-01-2 N2H4
 PRO V 127845-19-6
 SOL 64-17-5 EtOH

RX(43) OF 55 COMPOSED OF RX(3), RX(2), RX(4), RX(5), RX(6), RX(7), RX(8)
 RX(43) 2 B + 3 O ==> Y



7
STEPS
→



Y
YIELD 74%

RX(3) RCT B 56906-50-0
RGT I 334-88-3 CH2N2
PRO G 20972-45-6
SOL 60-29-7 Et2O

RX(2) RCT G 20972-45-6
PRO H 127845-14-1
NTE polyphosphoric acid

RX(4) RCT H 127845-14-1
RGT M 5470-11-1 H2NOH-HCl
PRO K 127845-15-2, L 127845-22-1
SOL 110-86-1 Pyridine

RX(5) RCT K 127845-15-2, O 108-24-7
RGT R 7772-99-8 SnCl2
PRO P 127845-16-3, Q 127845-17-4
SOL 108-24-7 Ac2O

RX(6) RCT Q 127845-17-4
RGT T 10025-87-3 POC13
PRO S 104958-38-5
SOL 95-47-6 o-Xylene

RX(7) RCT S 104958-38-5
RGT W 302-01-2 N2H4
PRO V 127845-19-6
SOL 64-17-5 EtOH

RX(8) RCT V 127845-19-6
RGT Z 7632-00-0 NaNO2
PRO Y 127845-20-9
SOL 64-19-7 AcOH, 7732-18-5 Water

L91 ANSWER 19 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

112:207807 CASREACT [Full-text](#)

TITLE:

N-aminophthalimide derivative-containing high-contrast dot-enhancing composition

INVENTOR(S):

Kojima, Yasuhiko; Pilot, John; Waxman, Burton H.

PATENT ASSIGNEE(S):

Polychrome Corp., USA; Dainippon Ink Chemical Industry Co.

SOURCE:

U.S., 13 pp.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

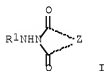
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4882261	A	19891121	US 1988-211980	19880627
JP 02052333	A	19900221	JP 1989-131228	19890524
AU 8936127	A	19900104	AU 1989-36127	19890607
AU 620101	B2	19920213		
EP 349274	A2	19900103	EP 1989-306523	19890627
EP 349274	A3	19900321		
EP 349274	B1	19940914		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ES 2058532	T3	19941101	ES 1989-306523	19890627
CA 1335241	C	19950418	CA 1989-604005	19890627
			US 1988-211980	19880627

PRIORITY APPLN. INFO.:

MARPAT 112:207807

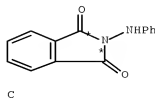
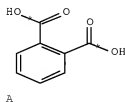
OTHER SOURCE(S):

GI



AB A dot-enhancing composition for use in a high-contrast neg.-working image-forming system contains a compound of the structure I (R1 = an aromatic group; Z = a substituted or unsubstituted aromatic nucleus, the 2 carbonyl groups are each bound to a different C atom of the aromatic nucleus). The composition, which may be incorporated into a lith Ag halide photog. emulsion, another hydrophilic colloid layer, a developer solution, or both, improves the d. and contrast of the images formed as well as provides harder, smoother, better formed dots for use in letterpress and offset lithog. plates.

RX(1) OF 1 A + B ==> C



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RX(1) RCT A 88-95-3, B 100-63-6
RGT D 7646-85-7 ZnCl2
PRO C 4879-16-0

L91 ANSWER 20 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 110:75426 CASREACT [Full-text](#)

TITLE: Pyridazine derivatives. VI. Synthesis and hypotensive activity of 3-hydrazinothieno[2,3-h]cinnoline and its derivatives

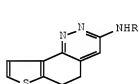
AUTHOR(S): Garcia-Dominguez, Neftali; Ravina, Enrique; Santana, Lourdes; Teran, Carmen; Garcia-Mera, Gerardo; Orallo, Francisco; Crespo, Manuel; Fontenla, Jose Angel
CORPORATE SOURCE: Lab. Pharm. Chem., Univ. Santiago de Compostela, Spain
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1988), 321(10), 735-8

CODEN: ARPMAS; ISSN: 0365-6233

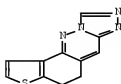
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

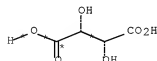


II

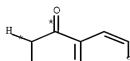
AB The title compound (I, R = NH2) was prepared from thiophene and succinic anhydride in 8 steps. Treatment of I (R = NH2) with HCO2H gave the triazolothienocinnoline II. I (R = NH2) had dose-dependent protracted antihypertensive activity which was significantly reduced in I (R = N:CMe2). Cyclization to II eliminated the antihypertensive activity.

RX(14) OF 45 COMPOSED OF RX(3), RX(5)

RX(14) K + F ==> R



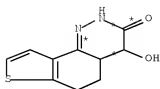
K



F

2
STEPS
→

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R
YIELD 92%

RX(3) RCT K 67-69-4

STAGE(1)

RGT H 7790-28-5 NaIO₄, I 7664-93-9 H₂SO₄
SOL 7732-18-5 Water

STAGE(2)

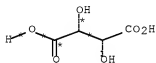
RCT F 13414-95-4
RGT L 1310-73-2 NaOH
SOL 64-17-5 EtOH

PRO G 118736-67-7

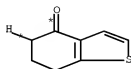
RX(5) RCT G 118736-67-7
RGT C 302-01-2 N₂H₄
PRO R 118736-68-8
SOL 64-17-5 EtOH

RX(23) OF 45 COMPOSED OF RX(3), RX(5), RX(7)

RX(23) K + F ==> T

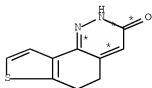


K



F

3
STEPS
→



T
YIELD 65%

RX(3) RCT K 87-65-4

STAGE(1)

RGT H 7790-28-5 NaIO₄, I 7664-93-9 H₂SO₄
 SOL 7732-18-5 Water

STAGE(2)

RCT F 13414-95-4
 RGT L 1310-73-2 NaOH
 SOL 64-17-5 EtOH

PRO G 118736-67-7

RX(5) RCT G 118736-67-7
 RGT C 302-01-2 N₂H₄
 PRO R 118736-68-8
 SOL 64-17-5 EtOH

RX(7) RCT R 118736-68-8
 RGT U 127-68-4 m-O₂NC₆H₄CO₂Na, L 1310-73-2 NaOH
 PRO T 118777-73-4
 SOL 7732-18-5 Water

L91 ANSWER 21 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 108:111649 CASREACT Full-text

TITLE: Microenvironmental effects of water-soluble polymers
 on the chemiluminescence of luminol and its analogs

AUTHOR(S): Karatani, Hajime

CORPORATE SOURCE: Fac. Text. Sci., Kyoto Inst. Technol., Kyoto, 606,
 Japan

SOURCE: Bulletin of the Chemical Society of Japan (1987),
 60(6), 2023-9

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

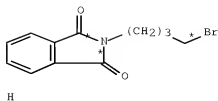
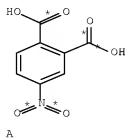
LANGUAGE: English

AB The effects of water-soluble polymers (WSPs), such as bovine serum albumin (BSA) and poly(ethylenimine) on chemiluminescence (CL) in an aqueous solution have been studied. The CL emission, particularly in the initial stage of the CL reaction, was strongly enhanced by increasing the concns. of these WSPs. This was attributed to the acceleration of the chemical reactions prior to the formation of the light-emitting species. BSA was also peculiar in that it could enhance CL under neutral pH conditions. It was suggested that these WSPs offered hydrophobic and basic microenvironments well suited to the CL reaction.

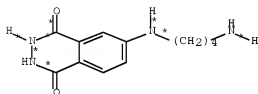
RX(60) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(6)

RX(60) A + H ==> K

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5
STEPS
→



K

RX(1) RCT A 610-27-5
PRO B 5466-84-2

RX(2) RCT B 5466-84-2
PRO C 41663-84-7

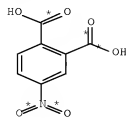
RX(3) RCT C 41663-84-7
RGT E 7647-01-0 HCl, F 7772-99-8 SnCl₂
PRO D 2307-00-8
SOL 7732-18-5 Water

RX(4) RCT H 5394-18-3, D 2307-00-8
PRO I 73819-85-9

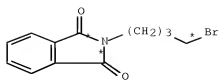
RX(6) RCT I 73819-85-9
RGT L 302-01-2 N₂H₄
PRO K 55612-28-0
SOL 64-17-5 EtOH

RX(70) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(11), RX(7)
RX(70) A + H + V ==> O

10/595943



A

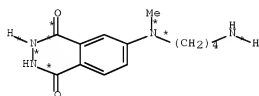


H



V

6
STEPS
→



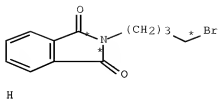
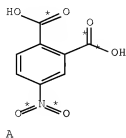
O

RX(1)	RCT	A 610-27-5
	PRO	B 5466-84-2
RX(2)	RCT	B 5466-84-2
	PRO	C 41663-84-7
RX(3)	RCT	C 41663-84-7
	RGT	E 7647-01-0 HCl, F 772-99-6 SnCl2
	PRO	D 2307-00-8
	SOL	7732-18-5 Water
RX(4)	RCT	H 5394-18-3, D 2307-00-8
	PRO	I 73819-85-9
RX(11)	RCT	I 73819-85-9, V 77-78-1
	PRO	N 113120-83-5
RX(7)	RCT	N 113120-83-5
	RGT	L 362-01-2 N2H4
	PRO	O 80344-69-0
	SOL	64-17-5 EtOH

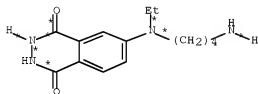
RX(71) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(12), RX(8)

10/595943

RX(71) A + H + W ==> Q



6
STEPS
→



RX(1) RCT A 610-27-5
 PRO B 5466-84-2

RX(2) RCT B 5466-84-2
 PRO C 41663-84-7

RX(3) RCT C 41663-84-7
 RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2
 PRO D 2307-00-8
 SOL 7732-18-5 Water

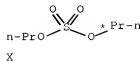
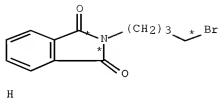
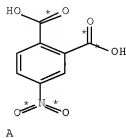
RX(4) RCT H 5394-18-3, D 2307-00-8
 PRO I 73819-85-9

RX(12) RCT I 73819-85-9, W 64-67-5
 PRO P 73819-87-1

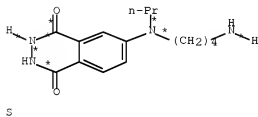
RX(8) RCT P 73819-87-1
 RGT L 302-01-2 N2H4
 PRO Q 66612-29-1
 SOL 64-17-5 EtOH

10/595943

RX(72) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13), RX(9)
 RX(72) A + H + X ==> S



6
 STEPS
 →

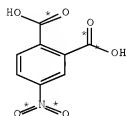


RX(1)	RCT	A 610-27-5
	PRO	B 5466-84-2
RX(2)	RCT	B 5466-84-2
	PRO	C 41663-84-7
RX(3)	RCT	C 41663-84-7
	RGT	E 7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO	D 2307-00-8
	SOL	7732-18-5 Water
RX(4)	RCT	H 5394-18-3, D 2307-00-8
	PRO	I 73819-85-9
RX(13)	RCT	I 73819-85-9, X 598-05-0
	PRO	R 113120-84-6
RX(9)	RCT	R 113120-84-6
	RGT	L 302-01-2 N2H4
	PRO	S 113120-84-6

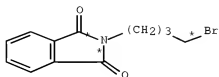
10/595943

SOL 64-17-5 EtOH

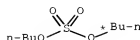
RX(73) OF 100 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(14), RX(10)
 RX(73) A + H + Y ==> U



A

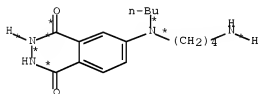


H



Y

6
 STEPS
 →



U

RX(1)	RCT A 616-27-5
	PRO B 5466-84-2
RX(2)	RCT B 5466-84-2
	PRO C 41663-84-7
RX(3)	RCT C 41663-84-7
	RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2
	PRO D 2307-00-8
	SOL 7732-18-5 Water
RX(4)	RCT H 5394-18-3, D 2307-00-8
	PRO I 73819-85-9
RX(14)	RCT I 73819-85-9, Y 625-22-9
	PRO T 113120-85-7
RX(10)	RCT T 113120-85-7

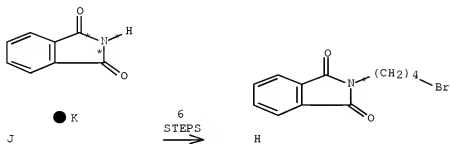
10/595943

RGT L 302-01-2 N2H4
 PRO U 113129-82-4
 SOL 64-17-5 EtOH

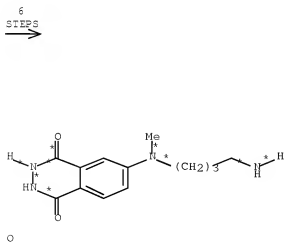
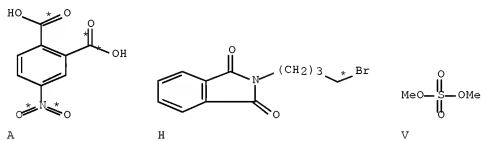
RX(92) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(11), RX(7)
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(11), RX(7)

...J ==> H...

... A + H + V ==> O



START NEXT REACTION SEQUENCE



RX(5) RCT J 1074-82-4
 PRO H 5394-18-3

 RX(1) RCT A 619-27-5
 PRO B 5466-84-2

 RX(2) RCT B 5466-84-2
 PRO C 41663-84-7

 RX(3) RCT C 41663-84-7
 RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2
 PRO D 2307-00-8
 SOL 7732-18-5 Water

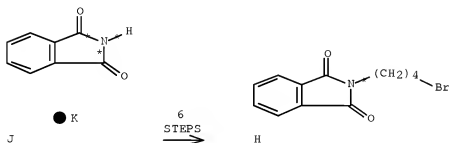
 RX(4) RCT H 5394-18-3, D 2307-00-8
 PRO I 73819-85-9

 RX(11) RCT I 73819-85-9, V 77-78-1
 PRO N 113120-83-5

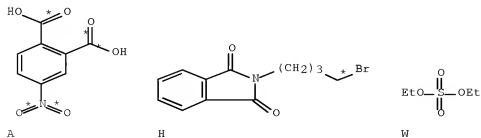
 RX(7) RCT N 113120-83-5
 RGT L 302-01-2 N2H4
 PRO O 80344-69-0
 SOL 64-17-5 EtOH

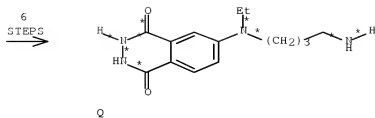
RX(93) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(12), RX(8)
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(12), RX(8)

...J ==> H...
 ... A + H + W ==> Q



START NEXT REACTION SEQUENCE





RX(5) RCT J 1074-82-4
PRO H 5394-18-3

RX(1) RCT A 610-27-5
PRO B 5466-84-2

RX(2) RCT B 5466-84-2
PRO C 41663-84-7

RX(3) RCT C 41663-84-7
RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2
PRO D 2307-00-8
SOL 7732-18-5 Water

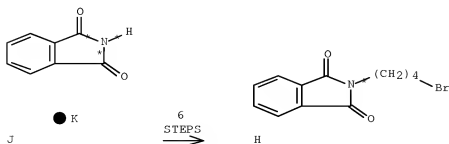
RX(4) RCT H 5394-18-3, D 2307-00-8
PRO I 73819-85-9

RX(12) RCT I 73819-85-9, W 64-67-5
PRO P 73819-87-1

RX(8) RCT P 73819-87-1
RGT L 302-01-2 N2H4
PRO Q 66612-29-1
SOL 64-17-5 EtOH

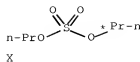
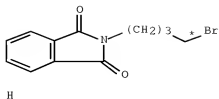
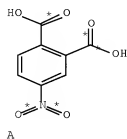
RX(94) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(13), RX(9)
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(13), RX(9)

...J ==> H...
... A + H + X ==> S

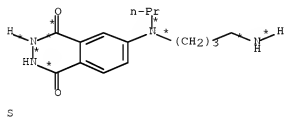


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START NEXT REACTION SEQUENCE



6
STEPS
→



RX(5)	RCT J 1074-82-4
	PRO H 5394-18-3
RX(1)	RCT A 610-27-5
	PRO B 5466-84-2
RX(2)	RCT B 5466-84-2
	PRO C 41663-84-7
RX(3)	RCT C 41663-84-7
	RGT E 7647-01-0 HCl, F 7732-99-8 SnCl2
	PRO D 2307-00-8
	SOL 7732-18-5 Water
RX(4)	RCT H 5394-18-3, D 2307-00-8
	PRO I 73819-85-9
RX(13)	RCT I 73819-85-9, X 598-05-0
	PRO R 113120-84-6
RX(9)	RCT R 113120-84-6
	RGT L 302-01-2 N2H4

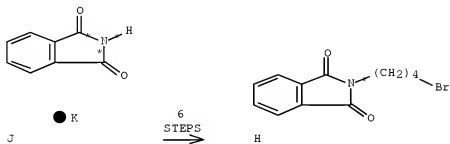
10/595943

PRO S 113120-81-3
 SOL 64-17-5 EtOH

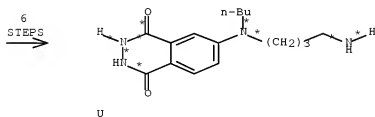
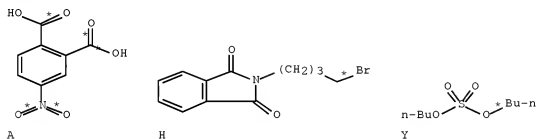
RX(95) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(14), RX(10)
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(14), RX(10)

...J ==> H...

... A + H + Y ==> J



START NEXT REACTION SEQUENCE



RX(5) RCT J 1074-82-4
 PRO H 5394-18-3

RX(1) RCT A 610-27-5
 PRO B 5466-84-2

RX(2) RCT B 5466-84-2
 PRO C 41663-84-7

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RX(3) RCT C 41663-84-7
 RGT E 7647-01-0 HCl, F 7772-89-8 SnCl2
 PRO D 2307-00-8
 SOL 7732-18-5 Water

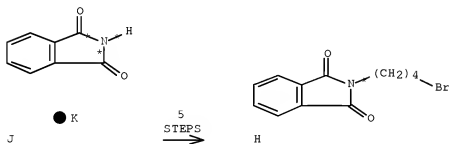
RX(4) RCT H 5394-18-3, D 2307-00-8
 PRO I 73819-85-9

RX(14) RCT I 73819-85-9, Y 625-22-9
 PRO T 113120-85-7

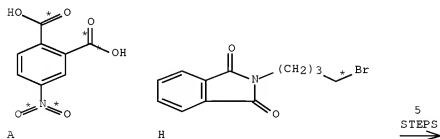
RX(10) RCT T 113120-85-7
 RGT L 302-01-2 N2H4
 PRO U 113120-82-4
 SOL 64-17-5 EtOH

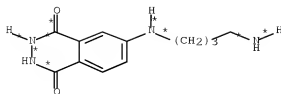
RX(96) OF 100 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(6)
 AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(6)

...J ==> H...
 ... A + H ==> K



START NEXT REACTION SEQUENCE





K

RX(5) RCT J 1074-82-4
PRO H 5394-18-3

RX(1) RCT A 610-27-5
PRO B 5466-84-2

RX(2) RCT B 5466-84-2
PRO C 41663-84-7

RX(3) RCT C 41663-84-7
RGT E 7647-01-0 HCl, F 7772-99-8 SnCl2
PRO D 2307-00-8
SOL 7732-18-5 Water

RX(4) RCT H 5394-18-3, D 2307-00-8
PRO I 73819-85-9

RX(6) RCT I 73819-85-9
RGT L 302-01-2 N2H4
PRO K 66612-28-0
SOL 64-17-5 EtOH

L91 ANSWER 22 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 108:21627 CASREACT [Full-text](#)

TITLE: Use of 2-(α -naphthylethyl)furan in diene
synthesis: an access to the derivatives of original
heterocycles

AUTHOR(S): Duval, O.; Gomes, L. Mavoungou

CORPORATE SOURCE: Lab. Chim. Org., Univ. Angers, Angers, 49000, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1987), (1),
131-42

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

GI

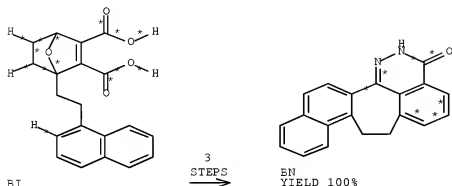
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Naphthyl Et furandicarboxylic acids (e.g., I, R = PhCH2CH2, α -naphthyl ethyl)
were prepared and converted to new heterocycles that include
dihydrooxonaphthocycloheptafuran II,
dioxotetrahydrobenzonaphthodicycloheptafuran III, and

dioxotetrahydrodinaphthodicycloheptafuran IV. A number of dihydronaphthocycloheptaphthalazines, e.g., V, prepared in connection with this study, are also described.

RX(172) OF 364 COMPOSED OF RX(26), RX(27), RX(28)

RX(172) BI ==> BN



RX(26) RCT BI 112036-40-5
RGT AQ 7664-38-2 H3PO4
PRO BJ 112036-41-6
SOL 64-19-7 AcOH

RX(27) RCT BJ 112036-41-6
RGT BL 7446-70-0 AlCl3, BC 7726-95-6 Br2
PRO BK 112036-42-7
SOL 79-34-5 Cl2HCCl2

RX(28) RCT BK 112036-42-7
RGT S 302-01-2 N2H4
PRO BN 112036-43-8
SOL 64-19-7 AcOH

L91 ANSWER 23 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 105:172383 CASREACT Full-text

TITLE: Conformationally restricted congeners of hypotensive and platelet aggregation inhibitors:

6-aryl-5-methyl-4,5-dihydro-3(2H)-pyridazinones

derived from 5H-indeno[1,2-c]pyridazine

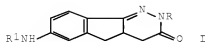
AUTHOR(S): Cignarella, Giorgio; Barlocco, Daniela; Pinna, Gerard A.; Loriga, Mario; Tofanetti, Odoardo; Germini, Mauro; Sala, Franca

CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Milano, Milan, 20131, Italy

SOURCE: Journal of Medicinal Chemistry (1986), 29(11), 2191-4
CODEN: JMCMAR; ISSN: 0022-2623

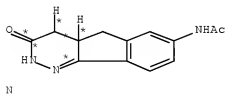
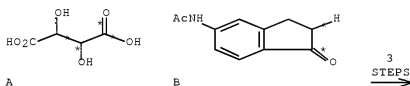
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



AB Indeno[1,2-c]pyridazin-3-ones I ($R = H, Me$; $R1 = H, Ac, COCHClMe$) were prepared as rigid congeners of hypotensive 6-aryl-5-methyl-4,5-dihydro-3(2H)-pyridazinones and tested as antihypertensive, antithrombotic, antiulcer, and antiinflammatory agents. Unlike the previously described 7-cyano derivative, which displayed only antiinflammatory action, the new series exhibited significant antihypertensive and antithrombotic properties. I ($R = H, R1 = H, Ac$) were found to be the most potent and long lasting in reducing the blood pressure in spontaneously hypertensive rats and in protecting mice from the induction of thrombosis. (ED₂₅ 2.60) I also exhibited antiinflammatory activity; and were highly effective in inhibiting indomethacin-induced ulcers in the rat.

RX(18) OF 26 COMPOSED OF RX(1), RX(2), RX(4)
 RX(18) A + B ==> N



RX(1) RCT A 87-65-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4
 SOL 7732-18-5 Water

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STAGE(2)

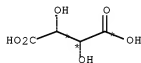
RCT B 58161-35-6
RGT F 1310-73-2 NaOH
SOL 64-17-5 EtOH

PRO C 103602-84-2

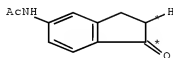
RX(2) RCT C 103602-84-2
RGT J 7440-66-6 Zn
PRO I 103422-85-1
SOL 64-19-7 AcOH

RX(4) RCT I 103422-85-1
RGT O 302-01-2 N2H4
PRO N 103422-54-4
SOL 64-17-5 EtOH

RX(19) OF 26 COMPOSED OF RX(1), RX(2), RX(7)
RX(19) A + B + T ==> U



A

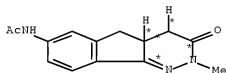


B



T

3
STEPS
→



U

RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4
SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6
RGT F 1310-73-2 NaOH
SOL 64-17-5 EtOH

PRO C 103602-84-2

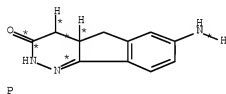
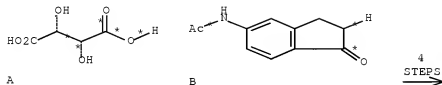
RX(2) RCT C 103602-84-2
RGT J 7440-66-6 Zn

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PRO I 103422-85-1
SOL 64-19-7 AcOH

RX(7) RCT I 103422-85-1, T 60-34-4
PRO U 103794-15-6
SOL 64-17-5 EtOH

RX(22) OF 26 COMPOSED OF RX(1), RX(2), RX(3), RX(5)
RX(22) A + B ==> P



RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4
SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6
RGT F 1310-73-2 NaOH
SOL 64-17-5 EtOH

PRO C 103602-84-2

RX(2) RCT C 103602-84-2
RGT J 7440-66-6 Zn
PRO I 103422-85-1
SOL 64-19-7 AcOH

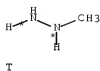
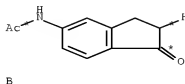
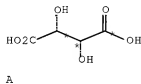
RX(3) RCT I 103422-85-1
RGT M 7647-01-0 HCl
PRO L 103422-62-4
SOL 7647-01-0 HCl, 7732-18-5 Water

RX(5) RCT L 103422-62-4
RGT O 302-01-2 N2H4

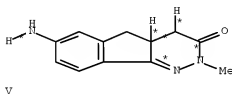
10/595943

PRO P 103422-53-3
SOL 64-17-5 EtOH

RX(23) OF 26 COMPOSED OF RX(1), RX(2), RX(3), RX(8)
RX(23) A + B + T ==> V



4
STEPS
→



RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7730-28-5 NaIO4
SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6
RGT F 1310-73-2 NaOH
SOL 64-17-5 EtOH

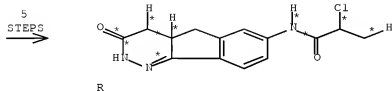
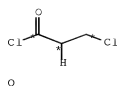
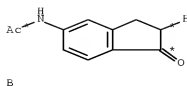
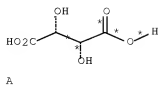
PRO C 103602-84-2

RX(2) RCT C 103602-84-2
RGT J 7440-66-6 Zn
PRO I 103422-85-1
SOL 64-19-7 AcOH

RX(3) RCT I 103422-85-1
RGT M 7647-01-0 HCl
PRO L 103422-62-4
SOL 7647-01-0 HCl, 7732-18-5 Water

RX(8) RCT L 103422-62-4, T 60-34-4
PRO V 103794-16-7
SOL 64-17-5 EtOH

RX(26) OF 26 COMPOSED OF RX(1), RX(2), RX(3), RX(5), RX(6)
RX(26) A + B + Q ==> R



RX(1) RCT A 87-69-4

STAGE(1)

RGT D 7664-93-9 H2SO4, E 7790-28-5 NaIO4

SOL 7732-18-5 Water

STAGE(2)

RCT B 58161-35-6

RGT F 1310-73-2 NaOH

SOL 64-17-5 EtOH

PRO C 103602-84-2

RX(2) RCT C 103602-84-2
RGT J 7440-66-6 Zn
PRO I 103422-85-1
SOL 64-19-7 AcOH

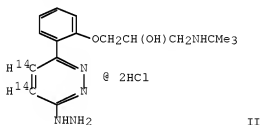
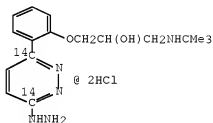
RX(3) RCT I 103422-85-1
RGT M 7647-01-0 HCl
PRO L 103422-62-4
SOL 7647-01-0 HCl, 7732-18-5 Water

RX(5) RCT L 103422-62-4
RGT O 302-01-2 N2H4
PRO P 103422-53-3
SOL 64-17-5 EtOH

RX(6) RCT P 103422-53-3, Q 625-36-5
PRO R 103602-84-1
SOL 108-88-3 PhMe

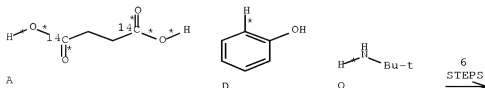
10/595943

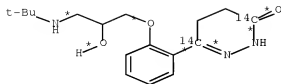
TITLE: Syntheses of carbon-14-labeled prizidilol dihydrochloride
 AUTHOR(S): Saunders, D.; Warrington, B. H.
 CORPORATE SOURCE: Smith Kline and French Res. Ltd., Welwyn/Hertfordshire, AL6 9AR, UK
 SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1985), 22(9), 869-81
 CODEN: JLCRD4; ISSN: 0362-4803
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Two syntheses of radiolabeled prizidilol-2HCl are described. A ten-stage synthesis gave [3,6-14C2]prizidilol-2HCl I in an overall yield of 0.91%. A later, alternative procedure led to [4,5-14C2]prizidilol-2HCl II with an overall radiochem. yield of 8%.

RX(71) OF 111 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)
 RX(71) A + D + O ==> Q



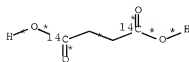


Q

RX(1)	RCT A 13613-74-6
	RGT C 7719-09-7 SOC12
	PRO B 42415-11-2
RX(2)	RCT B 42415-11-2, D 108-95-2
	RGT F 7446-79-0 AlCl3
	PRO E 103912-99-8
	SOL 79-34-5 C12HCCCHC12
RX(3)	RCT E 103912-99-8
	RGT I 7647-01-0 HCl
	PRO H 103913-00-4
	SOL 67-56-1 MeOH
RX(4)	RCT H 103913-00-4
	RGT L 584-08-7 K2CO3, M 3132-64-7 Epibromohydrin
	PRO K 103913-01-5
	SOL 78-93-3 EtOMe
RX(5)	RCT K 103913-01-5, O 75-64-9
	PRO P 103913-02-6
	SOL 67-56-1 MeOH
RX(6)	RCT P 103913-02-6
	RGT R 302-01-2 N2H4
	PRO Q 103913-03-7
	SOL 64-19-7 AcOH, 7732-18-5 Water

RX(74) OF 111 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7)

RX(74) A + D + O + 2 U ==> V



A



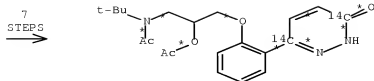
D



O



2 U



V

RX(1) RCT A 13613-74-6
RGT C 7719-09-7 SOC12
PRO B 42415-11-2

RX(2) RCT B 42415-11-2, D 108-95-2
RGT F 7446-70-0 AlCl3
PRO E 103912-99-8
SOL 79-34-5 Cl2HCCHC12

RX(3) RCT E 103912-99-8
RGT I 7647-01-0 HCl
PRO H 103913-00-4
SOL 67-56-1 MeOH

RX(4) RCT H 103913-00-4
RGT L 584-08-7 K2CO3, M 3132-64-7 Epibromohydrin
PRO K 103913-01-5
SOL 78-93-3 EtCOMe

RX(5) RCT K 103913-01-5, O 75-64-9
PRO P 103913-02-6
SOL 67-56-1 MeOH

RX(6) RCT P 103913-02-6
RGT R 302-01-2 N2H4
PRO Q 103913-03-7
SOL 64-19-7 AcOH, 7732-18-5 Water

RX(7) RCT Q 103913-03-7, U 108-24-7

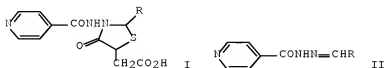
STAGE(1)
RGT L 584-08-7 K2CO3

STAGE(2)
RGT W 7726-95-6 Br2
SOL 64-19-7 AcOH

PRO V 103913-04-8

L91 ANSWER 25 OF 30 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 105:78865 CASREACT [Full-text](#)
TITLE: Studies on isoniazid derivatives. Preparation and
antimicrobial activity of
2-aryl-3-(pyridylcarbonyl)-5-carboxymethyl-4-
thiazolidinones
AUTHOR(S): Shah, R. R.; Mehta, R. D.; Parikh, A. R.

Dep. Chem., Saurashtra Univ., Rajkot, 360 005, India
Journal of the Indian Chemical Society (1985), 62(3),
255-7
CODEN: JICSAH; ISSN: 0019-4522

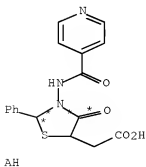
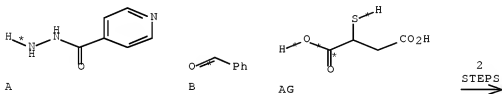
Journal
English

AB Fifteen thiazolidinones I [R = (un)substituted Ph, PhCH:CH, 2-furyl] were prepared by cyclization of the isoniazids II with thiomalic acid. Min. inhibitory concns. were determined for I and II against three bacteria.

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RX(31) OF 45 COMPOSED OF RX(1), RX(16)
RX(31)  A  +  B  +  AG  ==>  AH

```



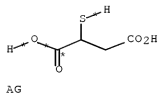
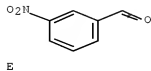
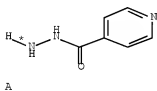
RX(1) RCT A 54-35-3, B 100-52-7

10/595943

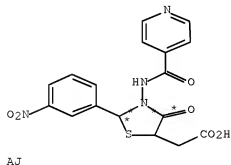
PRO C 533-02-8
SOL 67-56-1 MeOH

RX(16) RCT C 533-02-8, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AH 24327-74-3

RX(32) OF 45 COMPOSED OF RX(2), RX(17)
RX(32) A + E + AG ==> AJ



2
STEPS
→

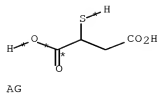
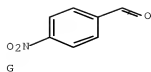
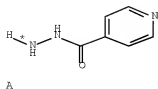


RX(2) RCT A 54-85-3, E 99-61-6
PRO F 16012-26-3
SOL 67-56-1 MeOH

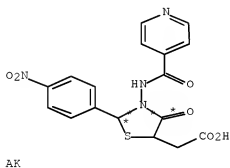
RX(17) RCT F 16012-26-3, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AJ 103706-31-6

RX(33) OF 45 COMPOSED OF RX(3), RX(18)
RX(33) A + G + AG ==> AK

10/595943



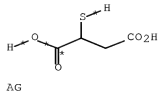
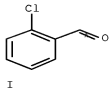
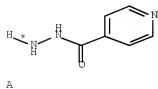
2
STEPS
→



RX(3) RCT A 54-85-3, G 555-16-8
PRO H 4813-07-4
SOL 67-56-1 MeOH

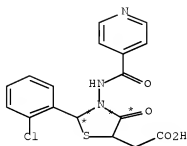
RX(18) RCT H 4813-07-4, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AK 163706-32-7

RX(34) OF 45 COMPOSED OF RX(4), RX(19)
RX(34) A + I + AG ==> AL



10/595943

2
STEPS
→

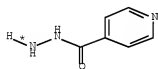


AL

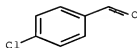
RX(4) RCT A 54-85-3, I 89-98-5
PRO J 16012-25-2
SOL 67-56-1 MeOH

RX(19) RCT J 16012-25-2, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AL 36195-32-1

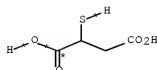
RX(35) OF 45 COMPOSED OF RX(5), RX(20)
RX(35) A + K + AG ==> AM



A



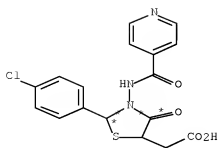
K



AG

2
STEPS
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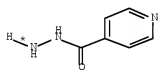


AM

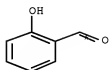
RX(5) RCT A 54-95-3, K 104-88-1
PRO L 6342-46-7
SOL 67-56-1 MeOH

RX(20) RCT L 6342-46-7, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AM 163719-50-5

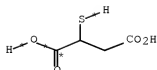
RX(36) OF 45 COMPOSED OF RX(6), RX(21)
RX(36) A + M + AG ==> AN



A



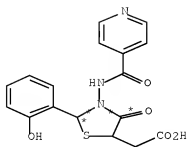
M



AG

2
STEPS
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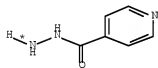


AN

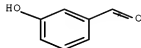
RX(6) RCT A 54-85-3, M 90-02-8
PRO N 495-84-1
SOL 67-56-1 MeOH

RX(21) RCT N 495-84-1, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AN 163706-33-8

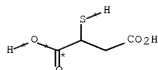
RX(37) OF 45 COMPOSED OF RX(7), RX(22)
RX(37) A + O + AG ==> AO



A



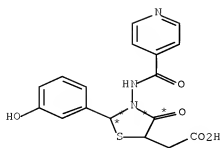
O



AG

2
STEPS
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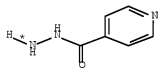


AO

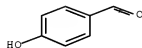
RX(7) RCT A 54-85-3, O 100-83-4
PRO P 840-80-2
SOL 67-56-1 MeOH

RX(22) RCT P 840-80-2, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AO 163706-34-9

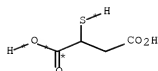
RX(38) OF 45 COMPOSED OF RX(8), RX(23)
RX(38) A + Q + AG ==> AP



A



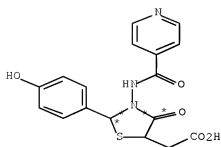
Q



AG

2
STEPS
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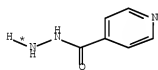


AP

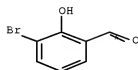
RX(8) RCT A 54-85-3, Q 123-08-0
PRO R 840-81-3
SOL 67-56-1 MeOH

RX(23) RCT R 840-81-3, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AP 163706-35-0

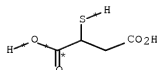
RX(39) OF 45 COMPOSED OF RX(9), RX(24)
RX(39) A + S + AG ==> AQ



A



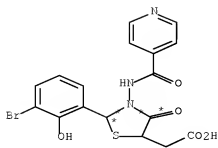
S



AG

2
STEPS
→

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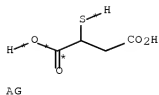
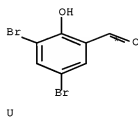
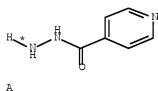


AQ

RX(9) RCT A 54-95-3, S 1829-34-1
PRO T 103706-30-5
SOL 67-56-1 MeOH

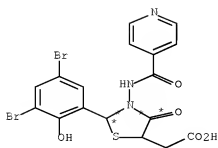
RX(24) RCT T 103706-30-5, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AQ 103706-36-1

RX(40) OF 45 COMPOSED OF RX(10), RX(25)
RX(40) A + U + AG ==> AR



2
STEPS
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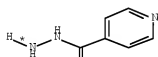


AR

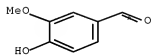
RX(10) RCT A 54-85-3, U 90-59-5
 PRO V 68639-25-8
 SOL 67-56-1 MeOH

RX(25) RCT V 68639-25-8, AG 70-49-5
 RGT AI 7646-85-7 ZnCl2
 PRO AR 163706-37-2

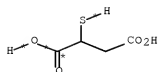
RX(41) OF 45 COMPOSED OF RX(11), RX(26)
 RX(41) A + W + AG ==> AS



A



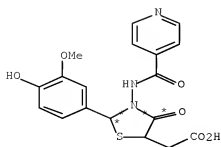
W



AG

2
 STEPS
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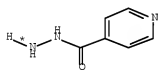


AS

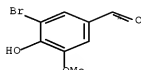
RX(11) RCT A 54-85-3, W 121-33-5
 PRO X 149-17-7
 SOL 67-56-1 MeOH

RX(26) RCT X 149-17-7, AG 70-49-5
 RGT AI 7646-85-7 ZnCl2
 PRO AS 163706-36-3

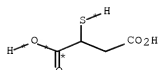
RX(42) OF 45 COMPOSED OF RX(12), RX(27)
 RX(42) A + Y + AG ==> AT



A



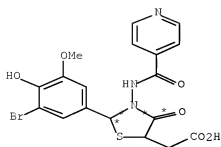
Y



AG

2
 STEPS
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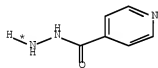


AT

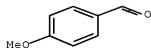
RX(12) RCT A 54-85-3, Y 2973-76-4
PRO Z 92160-05-9
SOL 67-56-1 MeOH

RX(27) RCT Z 92160-05-9, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AT 163706-39-4

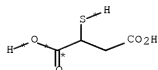
RX(43) OF 45 COMPOSED OF RX(13), RX(28)
RX(43) A + AA + AG ==> AU



A



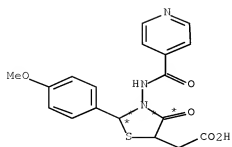
AA



AG

2
STEPS
→

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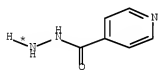


AU

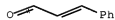
RX(13) RCT A 54-85-3, AA 123-11-5
 PRO AB 893-42-5
 SOL 67-56-1 MeOH

RX(28) RCT AB 893-42-5, AG 70-49-5
 RGT AI 7646-85-7 ZnCl2
 PRO AU 163706-40-7

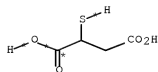
RX(44) OF 45 COMPOSED OF RX(14), RX(29)
 RX(44) A + AC + AG ==> AV



A



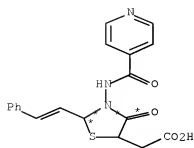
AC



AG

2
 STEPS
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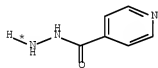


AV

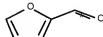
RX(14) RCT A 54-95-3, AC 104-55-2
PRO AD 4813-11-0
SOL 67-56-1 MeOH

RX(29) RCT AD 4813-11-0, AG 70-49-5
RGT AI 7646-85-7 ZnCl2
PRO AV 163706-41-8

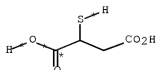
RX(45) OF 45 COMPOSED OF RX(15), RX(30)
RX(45) A + AE + AG ==> AW



A

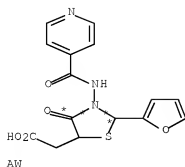


AE



AG

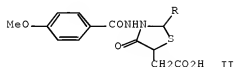
2
STEPS
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RX(15) RCT A 54-95-3, AE 98-01-1
 PRO AF 6956-53-2
 SOL 67-56-1 MeOH

RX(30) RCT AF 6956-53-2, AG 70-49-5
 RGT AI 7646-85-7 ZnCl2
 PRO AW 163706-42-9

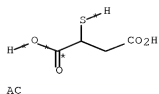
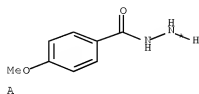
L91 ANSWER 26 OF 30 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 105:78864 CASREACT Full-text
 TITLE: Studies on antitubercular agents. Preparation of
 1-(4-methoxybenzoyl)-2-benzalhydrazines and
 2-aryl-3-(4-methoxybenzamido)-5-carboxymethyl-4-
 thiazolidinones
 AUTHOR(S): Patel, J. M.; Dave, M. P.; Langalia, N. A.; Thaker, K.
 A.
 CORPORATE SOURCE: Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India
 SOURCE: Journal of the Indian Chemical Society (1985), 62(3),
 254-5
 CODEN: JICSAH; ISSN: 0019-4522
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



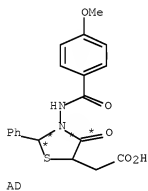
AB p-MeOC6H4CONHNH2 was condensed with RCHO [R = (un)substituted Ph, PhCH:CH] to give p-MeOC6H4CONHN:CHR (I) in 70-88% yield, which cyclized with HO2CCH2CH(SH)CO2H to give the thiazolidinones II in 55-76% yield. All I and II possess significant tuberculostatic activity at 30 µg/mL against Mycobacterium tuberculosis.

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RX(27) OF 39 COMPOSED OF RX(1), RX(14)
 RX(27) A + B + AC ==> AD



2
 STEPS

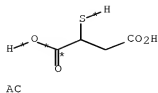
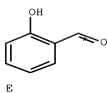
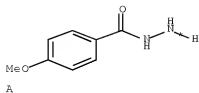


RX(1) RCT A 3290-99-1, B 100-52-7
 PRO C 51651-81-1
 SOL 64-17-5 EtOH

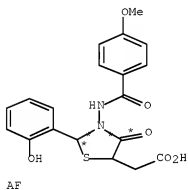
RX(14) RCT AC 70-49-5, C 51651-81-1
 RGT AE 7646-85-7 ZnCl2
 PRO AD 103635-31-0

RX(28) OF 39 COMPOSED OF RX(2), RX(15)
 RX(28) A + E + AC ==> AF

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STEPS
→

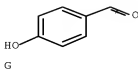
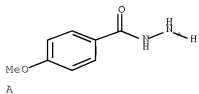


RX(2) RCT A 3290-99-1, E 90-02-8
PRO F 100969-61-7
SOL 64-17-5 EtOH

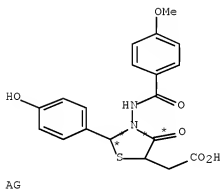
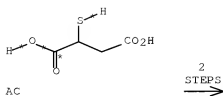
RX(15) RCT AC 70-49-5, F 100969-61-7
RGT AE 7646-85-7 ZnCl2
PRO AF 103635-32-1

RX(29) OF 39 COMPOSED OF RX(3), RX(16)

RX(29) A + G + AC ==> AG



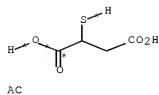
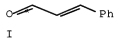
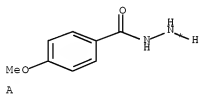
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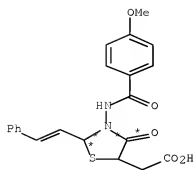


RX(3) RCT A 3290-99-1, G 123-08-0
PRO H 103635-23-0
SOL 64-17-5 EtOH

RX(16) RCT AC 70-49-5, H 103635-23-0
RGT AE 76-46-85-7 ZnCl2
PRO AG 103635-33-2

RX(30) OF 39 COMPOSED OF RX(4), RX(17)
RX(30) A + I + AC ==> AH



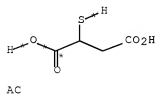
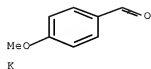
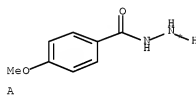


AH

RX(4) RCT A 3230-99-1, I 104-55-2
 PRO J 103635-24-1
 SOL 64-17-5 EtOH

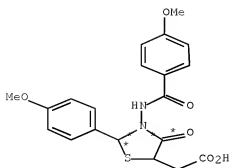
RX(17) RCT AC 70-49-5, J 103635-24-1
 RGT AE 7646-85-7 ZnCl2
 PRO AH 103635-34-3

RX(31) OF 39 COMPOSED OF RX(5), RX(18)
 RX(31) A + K + AC ==> AI



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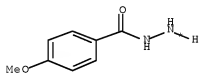
AI

RX(5) RCT A 3290-99-1, K 123-11-5
 PRO L 51771-21-2
 SOL 64-17-5 EtOH

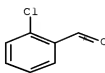
RX(18) RCT AC 70-49-5, L 51771-21-2
 RGT AE 7646-85-7 ZnCl2
 PRO AI 103635-35-4

RX(32) OF 39 COMPOSED OF RX(6), RX(19)

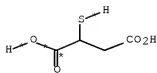
RX(32) A + M + AC ==> AJ



A



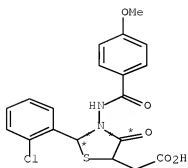
M



AC

2
 STEPS
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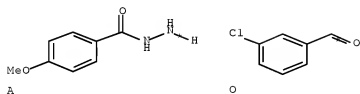


AJ

RX(6) RCT A 3290-99-1, M 89-98-5
 PRO N 103635-25-2
 SOL 64-17-5 EtOH

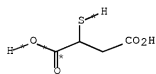
RX(19) RCT AC 70-49-5, N 103635-25-2
 RGT AE 7646-85-7 ZnCl2
 PRO AJ 103635-36-5

RX(33) OF 39 COMPOSED OF RX(7), RX(20)
 RX(33) A + O + AC ==> AK



A

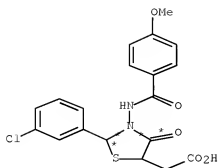
O



AC

2
 STEPS
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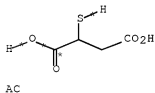
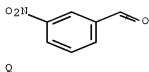
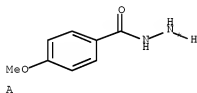
AK

RX(7) RCT A 3290-99-1, O 587-04-2
 PRO P 103635-26-3
 SOL 64-17-5 EtOH

RX(20) RCT AC 70-49-5, P 103635-26-3
 RGT AE 7646-85-7 ZnCl2
 PRO AK 103635-37-6

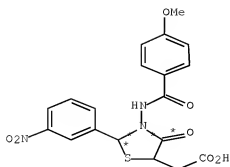
RX(34) OF 39 COMPOSED OF RX(8), RX(21)

RX(34) A + Q + AC ==> AL



2
 STEPS
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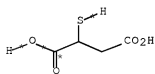
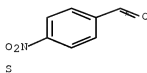
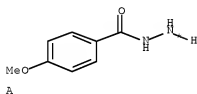
AL

RX(8) RCT A 3290-99-1, Q 99-61-6
 PRO R 103635-27-4
 SOL 64-17-5 EtOH

RX(21) RCT AC 70-49-5, R 103635-27-4
 RGT AE 7646-85-7 ZnCl2
 PRO AL 103635-38-7

RX(35) OF 39 COMPOSED OF RX(9), RX(22)

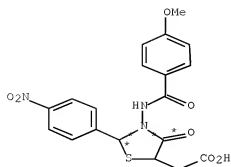
RX(35) A + S + AC ==> AM



AC

2
 STEPS
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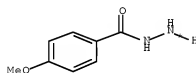
AM

RX(9) RCT A 3290-99-1, S 555-16-8
 PRO T 51771-23-4
 SOL 64-17-5 EtOH

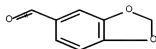
RX(22) RCT AC 70-49-5, T 51771-23-4
 RGT AE 7646-85-7 ZnCl2
 PRO AM 103635-39-6

RX(36) OF 39 COMPOSED OF RX(10), RX(23)

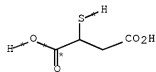
RX(36) A + U + AC ==> AM



A



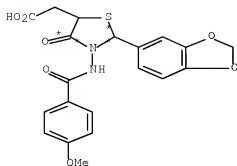
U



AC

2
 STEPS
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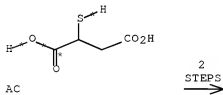
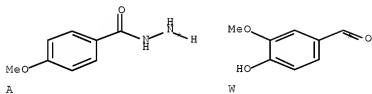
AN

RX(10) RCT A 3290-99-1, U 120-57-0
 PRO V 103635-28-5
 SOL 64-17-5 EtOH

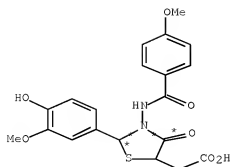
RX(23) RCT AC 70-49-5, V 103635-28-5
 RGT AE 7646-85-7 ZnCl2
 PRO AN 103635-40-1

RX(37) OF 39 COMPOSED OF RX(11), RX(24)

RX(37) A + W + AC ==> AG



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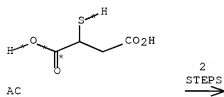
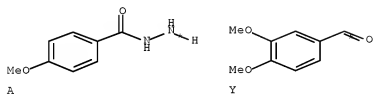
AO

RX(11) RCT A 3290-99-1, W 121-33-5
 PRO X 77218-64-5
 SOL 64-17-5 EtOH

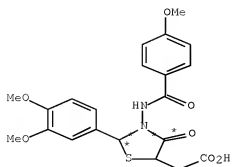
RX(24) RCT AC 70-49-5, X 77218-64-5
 RGT AE 7646-85-7 ZnCl2
 PRO AO 103635-41-2

RX(38) OF 39 COMPOSED OF RX(12), RX(25)

RX(38) A + Y + AC ==> AE



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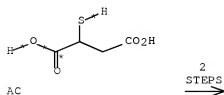
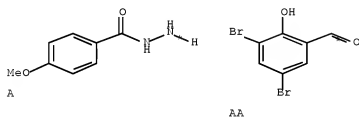


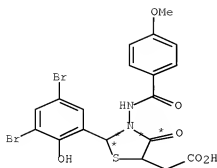
AP

RX(12) RCT A 3290-99-1, Y 120-14-9
 PRO Z 103635-29-6
 SOL 64-17-5 EtOH

RX(25) RCT AC 70-49-5, Z 103635-29-6
 RGT AE 7646-85-7 ZnCl2
 PRO AP 103635-42-3

RX(39) OF 39 COMPOSED OF RX(13), RX(26)
 RX(39) A + AA + AC ==> AQ





AQ

RX(13) RCT A 3290-99-1, AA 90-59-5
 PRO AB 103635-30-9
 SOL 64-17-5 EtOH

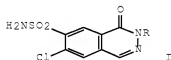
RX(26) RCT AC 70-49-5, AB 103635-30-9
 RGT AE 7646-85-7 ZnCl2
 PRO AQ 103635-43-4

L91 ANSWER 27 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 104:207223 CASREACT [Full-text](#)

TITLE: Synthesis, saludiuretic, and antihypertensive activity of 6,7-disubstituted 1(2H)- and 3,4-dihydro-1(2H)-phthalazinones
 Cherkez, S.; Herzig, J.; Yellin, H.
 CORPORATE SOURCE: Teva Pharm. Ind. Ltd., Tel-Aviv, 61 013, Israel
 SOURCE: Journal of Medicinal Chemistry (1986), 29(6), 947-59
 CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



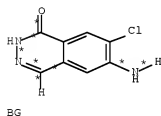
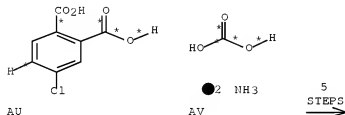
AB 6-Chloro-7-sulfamoyl-1(2H)-phthalazinones I (R = H, Me, PhCH2, m-CF3C6H4, furfuryl), four 7-chloro-6-sulfamoyl isomers (II), and their 3,4-dihydro derivs., combining structural features characteristic to furosemide and hydralazine, were prepared and their structure-activities relationships were studied. Preliminary screening in the rat shows that series I and dihydro derivs. exhibit diuretic and saluretic activity similar to that of chlorothiazide with, however, Na+/K+ ratios more favorable than chlorothiazide and furosemide. The compds. of series II and dihydro derivs. are practically inactive. All four series show initial antihypertensive activity lower than that of hydralazine. However, I (R = H, PhCH2) and II (R = H) dihydro

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derivative show a higher activity at 8 and/or 24 h after administration and thus may offer a unique combination of a "loop" diuresis with direct long-acting peripheral vasodilating effects.

RX(149) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28)

RX(149) AU + AV ==> BG



RX(23) RCT AU 89-20-3, AV 506-87-6
PRO AW 7147-90-2

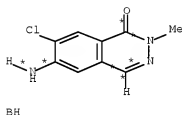
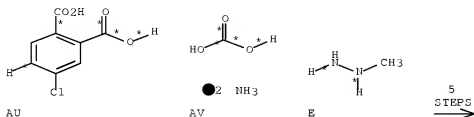
RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2
RGT C 362-01-2 N2H4
PRO BG 100448-46-2
SOL 7732-18-5 Water

RX(150) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29)
 RX(150) AU + AV + E ==> BH



RX(23) RCT AU 89-20-3, AV 506-87-6
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
 RGT BA 7697-37-2 HNO3
 PRO AZ 6015-57-2
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

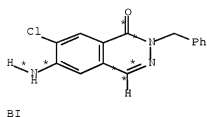
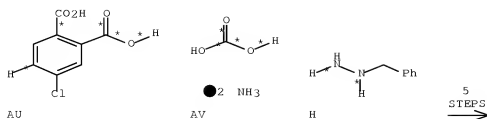
RX(26) RCT AZ 6015-57-2
 RGT BD 7772-39-8 SnCl2, M 7647-01-0 HCl
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4
 PRO BH 100448-48-4
 SOL 7732-18-5 Water

RX(151) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30)
 RX(151) AU + AV + H ==> EI

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RX(23) RCT AU 89-20-3, AV 506-87-6
 PRO AW 7147-90-2

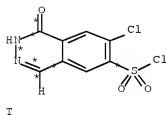
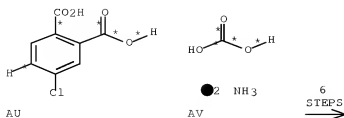
RX(25) RCT AW 7147-90-2
 RGT BA 7697-37-2 HNO3
 PRO AZ 6015-57-2
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt
 (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(30) RCT BE 100448-46-2, H 555-96-1
 PRO BI 100448-46-5
 SOL 7732-18-5 Water, 64-17-5 EtOH

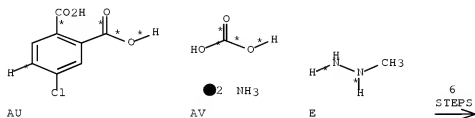
RX(161) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28), RX(32)
 RX(161) AU + AV ==> I



- RX(23) RCT AU 89-20-3, AV 506-87-6
 PRO AW 7147-90-2
- RX(25) RCT AW 7147-90-2
 RGT BA 7697-37-2 HNO₃
 PRO AZ 6015-57-2
 SOL 7664-93-9 H₂SO₄, 7732-18-5 Water
- RX(26) RCT AZ 6015-57-2
 RGT BD 7772-99-8 SnCl₂, M 7647-01-0 HCl
 PRO BC 5566-48-3
- RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water
- RX(28) RCT BE 100448-46-2
 RGT C 302-01-2 N₂H₄
 PRO BG 100448-47-3
 SOL 7732-18-5 Water
- RX(32) RCT BG 100448-47-3
- STAGE(1)
 RGT BM 7632-00-0 NaNO₂
 SOL 7732-18-5 Water
- STAGE(2)
 RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO₂
 SOL 64-19-7 AcOH

PRO T 100448-51-9

RX(162) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33)
 RX(162) AU + AV + E ==> W



RX(23) RCT AU 84-20-3, AV 506-87-6
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
 RGT BA 7697-37-2 HNO3
 PRO AZ 6015-57-2
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4
 PRO BH 100448-48-4
 SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

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STAGE(1)

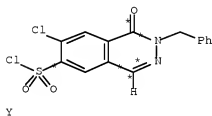
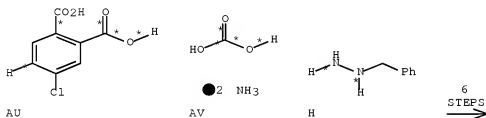
RGT BM 7632-00-0 NaNO₂, M 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO₂
SOL 64-19-7 AcOH

PRO W 100448-52-0

RX(163) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30), RX(34)
RX(163) AU + AV + H ==> Y



RX(23) RCT AU 89-20-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO₃
PRO AZ 6015-57-2
SOL 7664-93-9 H₂SO₄, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-39-8 SnCl₂, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

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RX(30) RCT BE 100448-46-2, H 555-56-4
 PRO BI 100448-49-5
 SOL 7732-18-5 Water, 64-17-5 EtOH

RX(34) RCT BI 100448-49-5

STAGE(1)

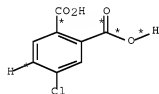
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
 SOL 7732-18-5 Water

STAGE(2)

RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2
 SOL 64-19-7 AcOH

PRO Y 100448-53-1

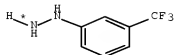
RX(164) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31)
 RX(164) AU + AV + BQ ==> BK



AU

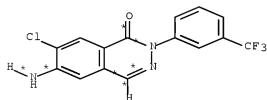


AV



BQ

6
 STEPS
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BK

RX(23) RCT AU 89-20-3, AV 506-87-6
 PRO AW 7147-90-2

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RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD ~~7772-99-8~~ SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

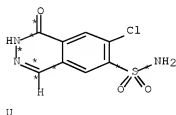
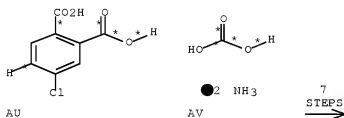
RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(39) RCT BE 100448-46-2, BQ ~~368-73-5~~
PRO BJ 100448-58-6
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(31) RCT BJ 100448-58-6
PRO BK ~~100448-50-8~~
SOL 67-68-5 DMSO

RX(177) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28), RX(32),
RX(7)

RX(177) AU + AV ==> U



RX(23) RCT AU ~~89-20-3~~, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2

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RGT BA 7697-37-2 HNO3
 PRO AZ 6015-57-2
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt
 (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2
 RGT C 302-01-2 N2H4
 PRO BG 100448-47-3
 SOL 7732-18-5 Water

RX(32) RCT BG 100448-47-3

STAGE(1)

RGT BM 7632-00-0 NaNO2
 SOL 7732-18-5 Water

STAGE(2)

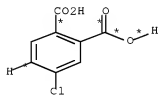
RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2
 SOL 64-19-7 AcOH

PRO T 100448-51-9

RX(7) RCT T 100448-51-9
 RGT V 7664-41-7 NH3
 PRO U 100448-31-5
 SOL 7664-41-7 NH3

RX(178) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33),
 RX(8)

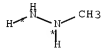
RX(178) AU + AV + E ==> X



AU

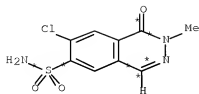


AV



E

7
 STEPS
 →



X

RX(23) RCT AU 89-29-3, AV 506-87-6
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
 RGT BA 7697-37-2 HNO3
 PRO AZ 6015-57-2
 SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
 RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4
 PRO BH 100448-48-4
 SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

STAGE(1)
 RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
 SOL 7732-18-5 Water

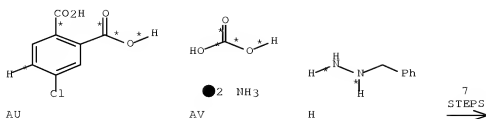
STAGE(2)
 RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2
 SOL 64-19-7 AcOH

PRO W 100448-52-0

RX(8) RCT W 100448-52-0
 RGT V 7664-41-7 NH3
 PRO X 100448-32-6
 SOL 7664-41-7 NH3

RX(179) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30), RX(34),
 RX(9)

RX(179) AU + AV + H ==> Z



RX(23) RCT AU 89-20-3, AV 506-87-6
 PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
 RGT BA 7697-37-2 HNO₃
 PRO AZ 6015-57-2
 SOL 7664-93-9 H₂SO₄, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
 RGT BD 7772-99-8 SnCl₂, M 7647-01-0 HCl
 PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(30) RCT BE 100448-46-2, H 555-96-1
 PRO BI 100448-49-5
 SOL 7732-18-5 Water, 64-17-5 EtOH

RX(34) RCT BI 100448-49-5

STAGE(1)
 RGT BM 7632-00-0 NaNO₂, M 7647-01-0 HCl
 SOL 7732-18-5 Water

STAGE(2)
 RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO₂
 SOL 64-19-7 AcOH

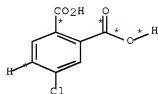
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PRO Y 100448-53-1

RX(9) RCT Y 100448-53-1
RGT V 7664-41-7 NH3
PRO Z 100448-53-7
SOL 7664-41-7 NH3

RX(180) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31),
RX(35)

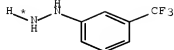
RX(180) AU + AV + BQ ==> AA



AU

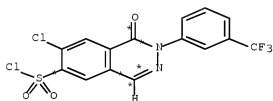


AV



BQ

7
STEPS
→



AA

RX(23) RCT AU 69-20-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

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RX(27) RCT BC 5566-48-3
 RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
 PRO BE 100448-46-2
 SOL 7732-18-5 Water

RX(39) RCT BE 100448-46-2, BQ 368-73-5
 PRO BJ 100448-58-6
 SOL 7732-18-5 Water, 64-17-5 EtOH

RX(31) RCT BJ 100448-58-6
 PRO BK 100448-50-8
 SOL 67-68-5 DMSO

RX(35) RCT BK 100448-50-8

STAGE(1)

RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
 SOL 7732-18-5 Water

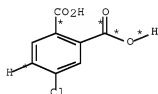
STAGE(2)

RGT BN 7756-89-6 CuCl, BO 7446-09-5 SO2
 SOL 64-19-7 AcOH

PRO AA 100448-54-2

RX(200) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31), RX(35), RX(10)

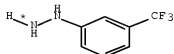
RX(200) AU + AV + BQ ==> AB



AU

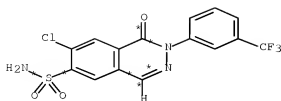


AV



BQ

8
 STEPS
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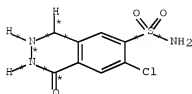
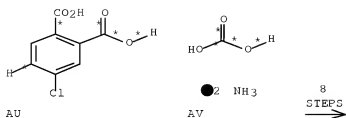
AB

- RX(23) RCT AU 89-29-3, AV 506-87-6
PRO AW 7147-90-2
- RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water
- RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-6 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3
- RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water
- RX(39) RCT BE 100448-46-2, BQ 368-78-5
PRO BJ 100448-58-6
SOL 7732-18-5 Water, 64-17-5 EtOH
- RX(31) RCT BJ 100448-58-6
PRO BK 100448-50-8
SOL 67-68-5 DMSO
- RX(35) RCT BK 100448-50-8
- STAGE(1)
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
SOL 7732-18-5 Water
- STAGE(2)
RGT BN 7758-99-6 CuCl, BO 7446-09-5 SO2
SOL 64-19-7 AcOH
- PRO AA 100448-54-2
- RX(10) RCT AA 100448-54-2
RGT V 7664-41-7 NH3
PRO AB 100448-34-8
SOL 7664-41-7 NH3

RX(201) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(28), RX(32),
RX(7), RX(17)

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RX(201) AU + AV ==> AK



RX(23) RCT AU 89-20-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(28) RCT BE 100448-46-2
RGT C 392-01-2 N2H4
PRO BG 100448-47-3
SOL 7732-18-5 Water

RX(32) RCT BG 100448-47-3

STAGE(1)
RGT BM 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(2)

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RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2
SOL 64-19-7 AcOH

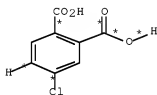
PRO T 100448-51-9

RX(7) RCT T 100448-51-9
RGT V 7664-41-7 NH3
PRO U 100448-31-5
SOL 7664-41-7 NH3

RX(17) RCT U 100448-31-5
RGT AE 16940-66-2 NaBH4
PRO AK 100448-41-7
SOL 111-96-6 (MeOCH2CH2)2O

RX(202) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33),
RX(8), RX(11)

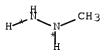
RX(202) AU + AV + E + Q ==> AC



AU



AV

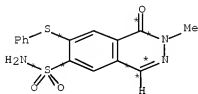


E



Q

8
STEPS
→



AC

RX(23) RCT AU 89-20-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3

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PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4
PRO BH 100448-48-4
SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

STAGE(1)

RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

RGT BN 7758-99-6 CuCl, BO 7446-09-5 SO2
SOL 64-19-7 AcOH

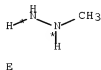
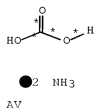
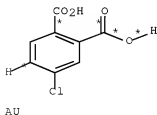
PRO W 100448-52-0

RX(8) RCT W 100448-52-0
RGT V 7664-41-7 NH3
PRO X 100448-32-6
SOL 7664-41-7 NH3

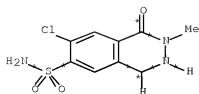
RX(11) RCT X 100448-32-6, Q 108-98-5
RGT S 144-55-8 NaHCO3
PRO AC 100448-35-9
SOL 7732-18-5 Water

RX(203) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(29), RX(33),
RX(8), RX(18)

RX(203) AU + AV + E ==> AL



8
STEPS
→



AL

RX(23) RCT AU 89-29-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(29) RCT BE 100448-46-2, E 60-34-4
PRO BH 100448-48-4
SOL 7732-18-5 Water

RX(33) RCT BH 100448-48-4

STAGE(1)
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT BN 7758-89-6 CuCl, BO 7446-09-5 SO2
SOL 64-19-7 AcOH

PRO W 100448-52-0

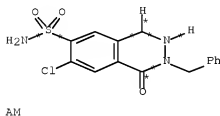
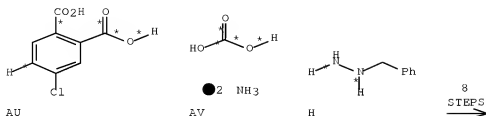
RX(8) RCT W 100448-52-0
RGT V 7664-41-7 NH3
PRO X 100448-32-6
SOL 7664-41-7 NH3

RX(18) RCT X 100448-32-6
RGT AE 16940-66-2 NaBH4
PRO AL 100448-42-8
SOL 111-96-6 (MeOCH2CH2)2O

RX(204) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(30), RX(34),

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RX(9), RX(19)
RX(204) AU + AV + H ==> AM



RX(23) RCT AU 89-20-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3
PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt (1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(30) RCT BE 100448-46-2, H 555-96-4
PRO BI 100448-49-5
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(34) RCT BI 100448-49-5

STAGE(1)
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

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RGT BN 7758-39-6 CuCl, BO 7446-09-5 SO2
SOL 64-19-7 AcOH

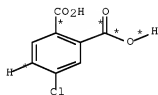
PRO Y 100448-53-1

RX(9) RCT Y 100448-53-1
RGT V 7664-41-7 NH3
PRO Z 100448-33-7
SOL 7664-41-7 NH3

RX(19) RCT Z 100448-33-7
RGT AE 16940-66-2 NaBH4
PRO AM 100448-43-9
SOL 111-96-6 (MeOCH2CH2)2O

RX(214) OF 215 COMPOSED OF RX(23), RX(25), RX(26), RX(27), RX(39), RX(31),
RX(35), RX(10), RX(20)

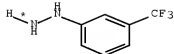
RX(214) AU + AV + BQ ==> AN



AU

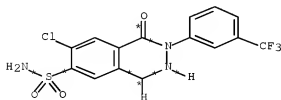


AV



BQ

9
STEPS
→



AN

RX(23) RCT AU 89-20-3, AV 506-87-6
PRO AW 7147-90-2

RX(25) RCT AW 7147-90-2
RGT BA 7697-37-2 HNO3

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PRO AZ 6015-57-2
SOL 7664-93-9 H2SO4, 7732-18-5 Water

RX(26) RCT AZ 6015-57-2
RGT BD 7772-99-8 SnCl2, M 7647-01-0 HCl
PRO BC 5566-48-3

RX(27) RCT BC 5566-48-3
RGT AR 7440-66-6 Zn, BF 18939-61-2 Sulfuric acid, copper(2+) salt
(1:?), G 1310-73-2 NaOH
PRO BE 100448-46-2
SOL 7732-18-5 Water

RX(39) RCT BE 100448-46-2, BQ 368-78-5
PRO BJ 100448-58-6
SOL 7732-18-5 Water, 64-17-5 EtOH

RX(31) RCT BJ 100448-58-6
PRO BK 100448-50-8
SOL 67-68-5 DMSO

RX(35) RCT BK 100448-50-8

STAGE(1)
RGT BM 7632-00-0 NaNO2, M 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT BN 7758-69-6 CuCl, BO 7446-09-5 SO2
SOL 64-19-7 AcOH

PRO AA 100448-54-2

RX(10) RCT AA 100448-54-2
RGT V 7664-41-7 NH3
PRO AB 100448-34-8
SOL 7664-41-7 NH3

RX(20) RCT AB 100448-34-8
RGT AE 16940-66-2 NaBH4
PRO AN 100448-44-0
SOL 111-96-6 (MeOCH2CH2)2O

L91 ANSWER 28 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 104:129829 CASREACT Full-text

TITLE: Synthesis and antitubercular activity of some
2-aryl-3-(4-chlorobenzamido)-5-substituted-4-
thiazolidinones

AUTHOR(S): Dave, M. P.; Patel, J. M.; Langalia, N. A.; Thaker, K.
A.

CORPORATE SOURCE: Dep. Chem., Bhavnagar Univ., Bhavnagar, 364 002, India
SOURCE: Journal of the Indian Chemical Society (1984), 61(10),
891-2

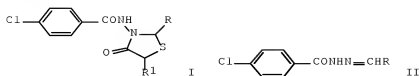
CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

LANGUAGE: English

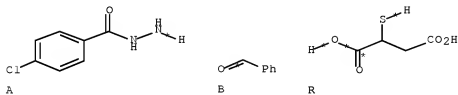
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10/595943

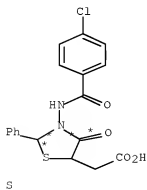


AB Title compds. I (R = Ph, C₆H₄NO₂-2, C₆H₄NO₂-4, C₆H₄OMe-4, C₆H₃(OMe)₂-3,4; R₁ = H, Me, CH₂CO₂H) were prepared by condensation of Schiff bases II with mercaptoalkanoic acids. I show antitubercular activity against Hs7Rv strain at 30 µg/mL in vitro.

RX(21) OF 33 COMPOSED OF RX(1), RX(8)
 RX(21) A + B + R ==> S



2
 STEPS
 →



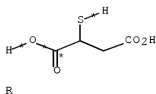
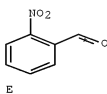
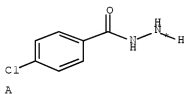
RX(1) RCT A 536-40-3, B 100-52-7

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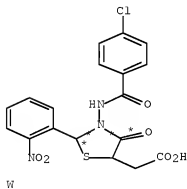
PRO C 31061-81-1
SOL 64-17-5 EtOH

RX(8) RCT R 70-49-5, C 31061-81-1
RGT T 7646-85-7 ZnCl2
PRO S 101125-20-6

RX(24) OF 33 COMPOSED OF RX(2), RX(11)
RX(24) A + E + R ==> W



2
STEPS
→

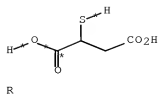
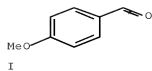
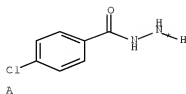


RX(2) RCT A 536-40-3, E 552-89-6
PRO F 62982-45-0
SOL 64-17-5 EtOH

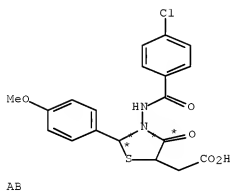
RX(11) RCT R 70-49-5, F 62982-45-0
RGT T 7646-85-7 ZnCl2
PRO W 101125-21-7

RX(30) OF 33 COMPOSED OF RX(4), RX(16)
RX(30) A + I + P ==> AE

10/595943



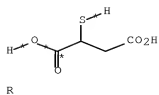
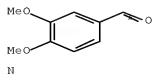
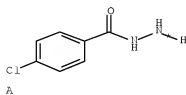
2
STEPS
→



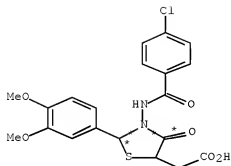
RX(4) RCT A 536-40-3, I 123-11-5
PRO J 51771-28-9
SOL 64-17-5 EtOH

RX(16) RCT R 70-49-5, J 51771-28-9
RGT T 7646-85-7 ZnCl2
PRO AB 101125-23-9

RX(32) OF 33 COMPOSED OF RX(6), RX(18)
RX(32) A + N + R ==> AB



2
STEPS
→



AD

RX(6) RCT A 536-40-3, N 120-14-9
PRO O 101125-30-8
SOL 64-17-5 EtOH

RX(18) RCT R 70-49-5, O 101125-30-8
RGT T 7646-85-7 ZnCl2
PRO AD 101125-24-0

L91 ANSWER 29 OF 30 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 100:139054 CASREACT [Full-text](#)

TITLE: 3-Aryl- and 3-(aryloxy)phthalic acids in the synthesis of fluorenones and xanthenes

AUTHOR(S): Oleinik, A. F.; Adamskaya, E. V.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, 119021, USSR

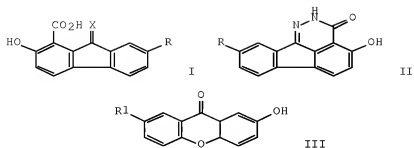
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1983), (11), 1537-9

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

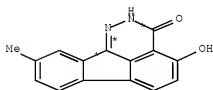
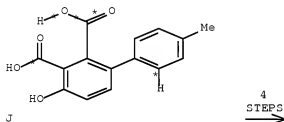
LANGUAGE: Russian

GI



AB Fluorenones I (R = Me, OH, X = O), prepared in 70 and 66% from the corresponding phthalic anhydride, were treated with N₂H₄.H₂O to give 76% I (X = NNH₂), which underwent intramol. cyclocondensation by heating in vacuo at 180-200° to give 42% II. Xanthenones III (R₁ = Me, H) were also obtained from the corresponding 3-phenoxyphthalic anhydride.

RX(32) OF 36 COMPOSED OF RX(4), RX(6), RX(1), RX(9)
 RX(32) J ==> F



YIELD 42%

RX(4) RCT J 84187-83-1
 PRO K 84207-12-5

RX(6) RCT K 84207-12-5

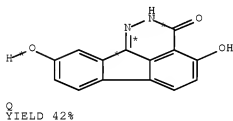
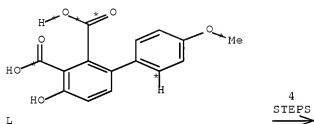
10/595943

RGT N 7446-70-0 AlCl3
PRO A 89450-81-7

RX(1) RCT A 89450-81-7
RGT C 302-01-2 N2H4, D 7732-18-5 Water
PRO B 89450-83-9
SOL 7732-18-5 Water

RX(9) RCT B 89450-83-9
PRO P 89450-85-1

RX(34) OF 36 COMPOSED OF RX(5), RX(7), RX(8), RX(10)
RX(34) L ==> Q



RX(5) RCT L 84185-84-2
PRO M 84185-72-8

RX(7) RCT M 84185-72-8
RGT N 7446-70-0 AlCl3
PRO G 89450-82-8

RX(8) RCT G 89450-82-8
RGT C 302-01-2 N2H4, D 7732-18-5 Water
PRO O 89450-84-0
SOL 7732-18-5 Water

RX(10) RCT O 89450-84-0
PRO Q 89450-86-2

10/595943

ACCESSION NUMBER:

TITLE:

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

GI

93:46557 CASREACT Full-text

Synthesis of the derivatives of

1-methoxyphenyl-3-hydroxypyridazin-6-ones. I.

Chlorination and substitution reactions

Baloniak, Sylwester; Linkowska, Ewa;

Zyczynska-Baloniak, Irena

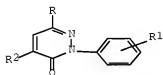
Inst. Chem. Anal., Sch. Med., Poznan, Pol.

Acta Poloniae Pharmaceutica (1979), 36(3), 301-6

CODEN: APPHAX; ISSN: 0001-6837

Journal

Polish



I, R=OH, R2=H, R1 as in text

II, R=Cl, R2=H, R1 as in text

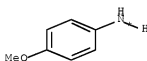
III, R=R2=Cl, R1 as in text

IV, R=Cl, R1 and R2 as in text

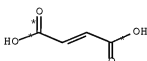
AB 3- And 4-MeOC6H4NHNH2-HCl refluxed with maleic anhydride in AcOH-AcONa gave I (R1 = 3- and 4-MeO, resp.). In preparation of I (R1 = 2-MeO), the intermediate 2-MeOC6H4NHNHCOCH:CHCO2H was isolated and cyclized with HCl. I were converted into the corresponding II by reaction with POCl3, whereas heating I in PCl5-POCl3 gave III. III heated with amines in DMF or alcs. gave 7 new IV (R2 = NHNH2, NEt2, 4-morpholinyl); IV (R2 = OMe) was obtained as the main product in the reaction of III with Et2NH.

RX(47) OF 66 COMPOSED OF RX(1), RX(2), RX(10), RX(16)

RX(47) A + E ==> AB



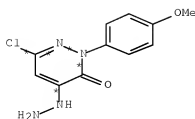
A



E

4
STEPS
→

10/595943



AB
YIELD 71%

RX(1) RCT A 104-94-9
RGT C 7782-77-6 HNO₂, D 7772-99-8 SnCl₂
PRO B 19501-58-7

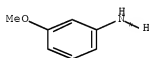
RX(2) RCT B 19501-58-7, E 6915-18-8
RGT G 7647-01-0 HCl
PRO F 60399-10-2

RX(10) RCT F 60399-10-2
RGT N 10025-87-3 POCl₃, R 10026-13-8 PCl₅
PRO S 73924-41-1

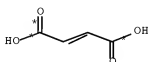
RX(16) RCT S 73924-41-1
RGT X 302-01-2 N₂H₄
PRO AB 73924-47-7

RX(61) OF 66 COMPOSED OF RX(20), RX(5), RX(9), RX(14)

RX(61) AH + E ==> Z

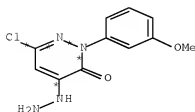


AH



E

4
STEPS
→



Z
YIELD 51%

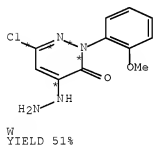
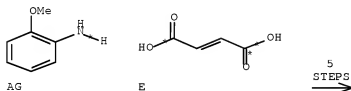
RX(20) RCT AH 536-90-3
 RGT C 7782-77-6 HNO₂, D 7772-99-8 SnCl₂
 PRO K 39232-91-2

 RX(5) RCT K 39232-91-2, E 6915-18-0
 RGT G 7647-01-0 HCl
 PRO L 73924-35-3

 RX(9) RCT L 73924-35-3
 RGT N 10025-87-3 POC13, R 10026-13-8 PC15
 PRO Q 73924-40-0

 RX(14) RCT Q 73924-40-0
 RGT X 302-01-2 N₂H₄
 PRO Z 73924-46-6

RX(66) OF 66 COMPOSED OF RX(19), RX(3), RX(4), RX(21), RX(12)
 RX(66) AG + E ==> W



RX(19) RCT AG 90-04-0
 RGT C 7782-77-6 HNO₂, D 7772-99-8 SnCl₂
 PRO H 6971-45-5

 RX(3) RCT H 6971-45-5, E 6915-18-0
 PRO I 344876-90-0

 RX(4) RCT I 344876-90-0

10/595943

RGT G 7647-01-0 HC1
PRO J 60399-12-4

RX(21) RCT J 60399-12-4
RGT N 10025-87-3 POC13, R 10026-13-8 PC15
PRO T 73924-39-7

RX(12) RCT T 73924-39-7
RGT X 302-01-2 N2H4
PRO W 73924-45-5

=> d his full

(FILE 'HOME' ENTERED AT 08:10:30 ON 17 OCT 2008)

FILE 'REGISTRY' ENTERED AT 08:15:23 ON 17 OCT 2008

ACT JAI943APRNS/A

```

L1      38 SEA ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/BI OR
      10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR 10026-12-7/B
      I OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/BI OR
      123-91-1/BI OR 13450-90-3/BI OR 22441-45-8/BI OR 3682-15-3/BI
      OR 521-31-3/BI OR 603-11-2/BI OR 67-64-1/BI OR 67-68-5/BI OR
      68-12-2/BI OR 7446-70-0/BI OR 7447-39-4/BI OR 7487-94-7/BI OR
      7550-45-0/BI OR 7637-07-2/BI OR 7646-79-9/BI OR 7646-85-7/BI
      OR 7647-18-9/BI OR 7697-37-2/BI OR 7705-07-9/BI OR 7705-08-0/BI
      OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/BI OR 7786-30-3/B
      I OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/BI OR 85-44-9/BI
      OR 872-50-4/BI)

```

ACT JAI943CATRNS/A

```

L2      28 SEA ABB=ON PLU=ON (10025-73-7/BI OR 10025-91-9/BI OR
      10026-07-0/BI OR 10026-10-5/BI OR 10026-11-6/BI OR 10026-12-7/B
      I OR 10049-06-6/BI OR 10108-64-2/BI OR 10294-34-5/BI OR
      13450-90-3/BI OR 22441-45-8/BI OR 7446-70-0/BI OR 7447-39-4/BI
      OR 7487-94-7/BI OR 7550-45-0/BI OR 7637-07-2/BI OR 7646-79-9/BI
      OR 7646-85-7/BI OR 7647-18-9/BI OR 7705-07-9/BI OR 7705-08-0/B
      I OR 7718-54-9/BI OR 7758-89-6/BI OR 7784-34-1/BI OR 7786-30-3/
      BI OR 7787-47-5/BI OR 7787-60-2/BI OR 7789-48-2/BI)

```

ACT JAI943SOLRNS/A

```

L3      5 SEA ABB=ON PLU=ON (123-91-1/BI OR 67-64-1/BI OR 67-68-5/BI
      OR 68-12-2/BI OR 872-50-4/BI)

```

```

L4      5 SEA ABB=ON PLU=ON L1 NOT (L2 OR L3)
      D SCA

```

FILE 'ZCAPLUS' ENTERED AT 08:17:38 ON 17 OCT 2008

ACT JAI943APP/A

```

L5      1 SEA ABB=ON PLU=ON US2006-595943/AP
      D SCA

```

FILE 'CASREACT' ENTERED AT 08:22:57 ON 17 OCT 2008

```

L6      STRUCTURE UPLOADED
L7      6 SEA SSS SAM L6 ( 45 REACTIONS)
      D SCA
      D STAT QUE
L8      446 SEA SSS FUL L6 ( 4732 REACTIONS)
      SAVE TEMP L8 JAI943STR6L/A

```

FILE 'REGISTRY' ENTERED AT 08:30:49 ON 17 OCT 2008

```

L9      23 SEA ABB=ON PLU=ON L2 AND M/ELS
L10     5 SEA ABB=ON PLU=ON L2 NOT L9
      D SCA
L11     23 SEA ABB=ON PLU=ON L9 AND X/ELS

```

D SCA

FILE 'CASREACT' ENTERED AT 08:32:57 ON 17 OCT 2008
 L12 TRA PLU=ON L8 1- RX : 5601 TERMS

FILE 'REGISTRY' ENTERED AT 08:37:17 ON 17 OCT 2008
 L13 5601 SEA ABB=ON PLU=ON L12/RN
 L14 11 SEA ABB=ON PLU=ON L13 AND L2
 D SCA
 L15 348 SEA ABB=ON PLU=ON L13 AND (M/ELS OR B/ELS OR AS/ELS OR
 TE/ELS OR AT/ELS)
 L16 97 SEA ABB=ON PLU=ON L15 AND X/ELS
 L17 86 SEA ABB=ON PLU=ON L16 NOT L14
 L18 62 SEA ABB=ON PLU=ON L17 AND C/ELS
 L19 24 SEA ABB=ON PLU=ON L17 NOT L18
 D SCA

FILE 'CAPLUS' ENTERED AT 08:45:57 ON 17 OCT 2008
 E LEWIS ACIDS+ALL/CT
 E LEWIS ACIDS+MAX/CT

FILE 'CASREACT' ENTERED AT 08:47:18 ON 17 OCT 2008
 L20 2766 SEA ABB=ON PLU=ON LEWIS ACID?/CW
 L21 9688 SEA ABB=ON PLU=ON LEWIS ACID?/BI,NTE
 L22 7 SEA ABB=ON PLU=ON L8 AND (L20 OR L21)
 D SCA
 L23 134073 SEA ABB=ON PLU=ON L16
 L24 103 SEA ABB=ON PLU=ON L23 (L) L8
 L25 STRUCTURE UPLOADED
 L26 15 SEA SUB=L8 SSS SAM L25 (304 REACTIONS)
 L27 331 SEA SUB=L8 SSS FUL L25 (3351 REACTIONS)
 L28 66 SEA ABB=ON PLU=ON L27 (L) L23

FILE 'REGISTRY' ENTERED AT 08:57:03 ON 17 OCT 2008
 L29 35 SEA ABB=ON PLU=ON L14 OR L19
 D SCA

FILE 'CASREACT' ENTERED AT 09:01:59 ON 17 OCT 2008
 L30 106670 SEA ABB=ON PLU=ON L29
 L31 15382 SEA ABB=ON PLU=ON L18/CAT
 L32 53 SEA ABB=ON PLU=ON L27 (L) L30
 L33 6 SEA ABB=ON PLU=ON L27 (L) L31
 L34 57 SEA ABB=ON PLU=ON L32 OR L33
 L35 STRUCTURE UPLOADED
 L36 12 SEA SUB=L8 SSS SAM L35 (283 REACTIONS)
 L37 239 SEA SUB=L8 SSS FUL L35 (2506 REACTIONS)
 L38 42 SEA ABB=ON PLU=ON L37 (L) L30
 L39 5 SEA ABB=ON PLU=ON L37 (L) L31
 L40 45 SEA ABB=ON PLU=ON L38 OR L39
 D SCA

FILE 'STNGUIDE' ENTERED AT 09:19:14 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 09:21:09 ON 17 OCT 2008

FILE 'REGISTRY' ENTERED AT 09:24:00 ON 17 OCT 2008
 L41 1 SEA ABB=ON PLU=ON L13 AND NB/ELS
 D SCA
 D RN

```

FILE 'CASREACT' ENTERED AT 09:25:01 ON 17 OCT 2008
L42      152 SEA ABB=ON PLU=ON 10026-12-7
L43      1 SEA ABB=ON PLU=ON L42 (L) L8
          D SCA
L44      50 SEA ABB=ON PLU=ON L40 OR L22
          D OCC 1- L44
          D COST
          D HIT 30

FILE 'REGISTRY' ENTERED AT 09:35:28 ON 17 OCT 2008
L45      2 SEA ABB=ON PLU=ON L29 AND B/ELS
          D SCA
L46      1 SEA ABB=ON PLU=ON L45 NOT F/ELS
L47      1 SEA ABB=ON PLU=ON L45 NOT L46
          D SCA
          D RN

FILE 'CASREACT' ENTERED AT 09:36:56 ON 17 OCT 2008
L*** DEL 0 S 16872-11-0 R
L48      2084 SEA ABB=ON PLU=ON 16872-11-0
L49      1 SEA ABB=ON PLU=ON L48 (L) L38
L50      0 SEA ABB=ON PLU=ON L48 (L) L39
L51      49 SEA ABB=ON PLU=ON L44 NOT L49

FILE 'REGISTRY' ENTERED AT 09:37:47 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 09:38:15 ON 17 OCT 2008
          D OCC L22 1-
          D OCC L38 1-
          D OCC L39 1-
          D OCC 1- L38
          D FHIT L38 3
          D FHIT L38 4
L52      446 SEA ABB=ON PLU=ON L8/COM
L53      239 SEA ABB=ON PLU=ON L37/COM
L54      STRUCTURE UPLOADED
L55      12 SEA SUB=L8 SSS SAM L54 ( 283 REACTIONS)
L56      239 SEA SUB=L8 SSS FUL L54 ( 2506 REACTIONS)
L57      42 SEA ABB=ON PLU=ON L56 (L) L30
L58      5 SEA ABB=ON PLU=ON L56 (L) L31
          D OCC L57 1-
          D FHIT 5 L38
          D FHIT 6 L38
          D FHIT 7 L38
          D FHIT 17 L38
          D FHIT 21 L38
L59      STRUCTURE UPLOADED
L60      9 SEA SUB=L8 SSS SAM L59 ( 136 REACTIONS)
          D SCA
L61      163 SEA SUB=L8 SSS FUL L59 ( 1426 REACTIONS)
L62      1 SEA ABB=ON PLU=ON L61 AND L20
L63      1 SEA ABB=ON PLU=ON L61 AND L21
L64      30 SEA ABB=ON PLU=ON L61 (L) L30
L65      2 SEA ABB=ON PLU=ON L61 (L) L31
L66      30 SEA ABB=ON PLU=ON (L62 OR L63 OR L64 OR L65)
          D OCC 1-
          D COST
          D SCA L65
          D HIT L65 1
L67      12 SEA ABB=ON PLU=ON L64 AND NS>5

```

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L68      1 SEA ABB=ON  PLU=ON  L43 AND L66
L69      1159 SEA ABB=ON  PLU=ON  NIOBIUM/BI,CW,NTE
L70      1 SEA ABB=ON  PLU=ON  L69 AND L61
L71      0 SEA ABB=ON  PLU=ON  L70 AND L49
L72      1 SEA ABB=ON  PLU=ON  L70 AND L43

FILE 'CAPLUS' ENTERED AT 10:13:14 ON 17 OCT 2008
L73      643 SEA ABB=ON  PLU=ON  LOPES C7/AU
L74      331 SEA ABB=ON  PLU=ON  LOPES R7/AU
L75      368 SEA ABB=ON  PLU=ON  CARDOSO J2/AU
L76      2399 SEA ABB=ON  PLU=ON  SILVA J2/AU OR DA SILVA J2/AU OR DASILVA
      J2/AU
L77      1104 SEA ABB=ON  PLU=ON  FERREIRA L7/AU
L*** DEL 28 S L73 AND L74-L76
L*** DEL 22 S L74 AND L75-L78
L78      28 SEA ABB=ON  PLU=ON  L73 AND (L74 OR L75 OR L76 OR L77)
L79      8 SEA ABB=ON  PLU=ON  L74 AND (L75 OR L76 OR L77)
L80      2 SEA ABB=ON  PLU=ON  L75 AND (L76 OR L77)
L81      16 SEA ABB=ON  PLU=ON  L76 AND L77
L82      8 SEA ABB=ON  PLU=ON  L78 AND (L79 OR L80 OR L81)
L83      0 SEA ABB=ON  PLU=ON  L79 AND (L80 OR L81)
L84      0 SEA ABB=ON  PLU=ON  L80 AND L81
L85      8 SEA ABB=ON  PLU=ON  (L82 OR L83 OR L84)
L86      446 SEA ABB=ON  PLU=ON  L8
L87      3 SEA ABB=ON  PLU=ON  L86 AND (L73 OR L74 OR L75 OR L76 OR L77)

FILE 'REGISTRY' ENTERED AT 10:17:11 ON 17 OCT 2008

FILE 'CAPLUS' ENTERED AT 10:17:14 ON 17 OCT 2008
      D STAT QUE L85
      D STAT QUE L87

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:17:32 ON 17 OCT 2008
L88      4 SEA ABB=ON  PLU=ON  L85

FILE 'ZCAPLUS' ENTERED AT 10:17:43 ON 17 OCT 2008

FILE 'CAPLUS' ENTERED AT 10:17:48 ON 17 OCT 2008
L89      10 SEA ABB=ON  PLU=ON  L85 OR L87

FILE 'CAPLUS, MEDLINE, EMBASE, WPIX' ENTERED AT 10:18:05 ON 17 OCT 2008
L90      11 DUP REM L89 L88 (3 DUPLICATES REMOVED)
      ANSWERS '1-10' FROM FILE CAPLUS
      ANSWER '11' FROM FILE MEDLINE
      D IBIB ABS L90 1-10
      D IALL L90 11

FILE 'REGISTRY' ENTERED AT 10:18:43 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 10:18:46 ON 17 OCT 2008
      D STAT QUE L43
      D IBIB ABS HIT L43 1

FILE 'REGISTRY' ENTERED AT 10:19:27 ON 17 OCT 2008

FILE 'CASREACT' ENTERED AT 10:19:29 ON 17 OCT 2008
      D STAT QUE L62
      D STAT QUE L63
      D STAT QUE L64
      D STAT QUE L65

```


L91 30 SEA ABB=ON PLU=ON L62 OR L63 OR L64 OR L65
 D IBIB ABS HIT L91 1-30

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5

DICTIONARY FILE UPDATES: 15 OCT 2008 HIGHEST RN 1061881-29-5

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE ZCAPLUS

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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17

FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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FILE CONTENT:1840 - 12 Oct 2008 VOL 149 ISS 16

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*

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FILE COVERS 1907 - 17 Oct 2008 VOL 149 ISS 17

FILE LAST UPDATED: 16 Oct 2008 (20081016/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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FILE STINGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Oct 10, 2008 (20081010/UP).

FILE MEDLINE

FILE LAST UPDATED: 16 Oct 2008 (20081016/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

MEDLINE Accession Numbers (ANs) for records from 1950-1977 have been converted from 8 to 10 digits. Searches using an 8 or 10 digit AN will retrieve the same record. The 10-digit ANs can be expanded, searched, and displayed in all records from 1949 to the present.

FILE EMBASE
FILE COVERS 1974 TO 17 Oct 2008 (20081017/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE BIOSIS
FILE COVERS 1926 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 15 October 2008 (20081015/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX
FILE LAST UPDATED: 13 OCT 2008 <20081013/UP>
MOST RECENT UPDATE: 200865 <200865/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
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>>> IPC Reform backfile reclassifications have been loaded to the end of June 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC, 20080401/UPIC and 20080701/UPIC.
ECLA reclassifications to June and US national classifications to the end of April 2008 have also been loaded. Update dates 20080401 and 20080701/UPEC and /UPNC have been assigned to these. <<<

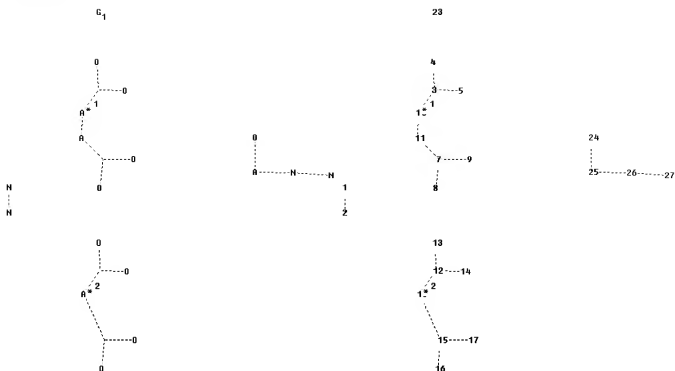
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>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

Uploading L6.str



```

chain nodes :
3 4 5 7 8 9 12 13 14 15 16 17 23 24
ring/chain nodes :
1 2 10 11 18 25 26 27
chain bonds :
3-4 3-5 3-10 7-8 7-9 7-11 12-13 12-14 12-18 15-16 15-17 15-18 24-25

ring/chain bonds :
1-2 10-11 25-26 26-27
exact/norm bonds :
1-2 3-4 3-5 3-10 7-8 7-9 7-11 10-11 12-13 12-14 12-18 15-16 15-17 15-18
24-25 25-26 26-27

```

G1:[*1],[*2]

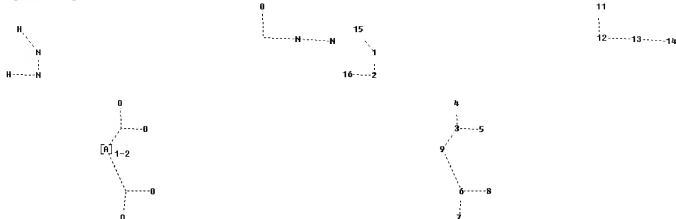
Connectivity :

```

3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
7:3 E exact RC ring/chain 8:1 E exact RC ring/chain 9:1 E exact RC ring/chain
12:3 E exact RC ring/chain
13:1 E exact RC ring/chain 14:1 E exact RC ring/chain 15:3 E exact RC ring/chain
16:1
E exact RC ring/chain 17:1 E exact RC ring/chain 24:1 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS
fragments assigned product role:
containing 24
fragments assigned reactant/reagent role:
containing 1
containing 23

```

Uploading L59.str



```

chain nodes :
4 5 7 8 11 15 16
ring/chain nodes :
1 2 3 6 9 12 13 14
chain bonds :
1-15 2-16 3-4 3-5 6-7 6-8 11-12
ring/chain bonds :
1-2 3-9 6-9 12-13 13-14
exact/norm bonds :
1-2 1-15 2-16 3-4 3-5 3-9 6-7 6-8 6-9 11-12 12-13 13-14

```

```

Connectivity :
3:3 E exact RC ring/chain 4:1 E exact RC ring/chain 5:1 E exact RC ring/chain
6:3 E exact RC ring/chain 7:1 E exact RC ring/chain 8:1 E exact RC ring/chain
11:1 E exact RC ring/chain

```

```

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS
fragments assigned reactant role:
containing 3
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
reaction site bonds:
12-13:CC
node mappings:
3:12 1:13

```

=>